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Ogawa, Shun

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Study on non-equilibrium quasi-stationary states for Hamiltonian systems with long-range interaction

Shun Ogawa

Department of Applied Mathematics and Physics,
Graduate School of Informatics, Kyoto University,
606-8501 Kyoto, Japan

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Chapter 1

Introduction

In both equilibrium and non-equilibrium states, Hamiltonian systems with long-range interaction [DRAW2002, CDR2009] show macroscopic behavior that differs markedly from ones with short-range interaction, which satisfy assumptions of both additivity and extensivity so that the equilibrium statistical mechanics works. For instance, the additivity of the energy is necessary for deriving the canonical ensemble of a system in question from the microcanonical ensemble of a larger system consisting of the system and a huge bath system [LL1968]. The statistical physics of systems with long-range interaction has begun to attract notice, and it has not been so well explored as that of short-range interacting systems, although long-range interaction systems are observed in various scales in nature as stellar systems [BT2008], plasma systems [Ich1973, LP1981], two-dimensional point vortex systems [Ons1949], cold atoms, and magnetic dipoles [DRAW2002, CDR2009, DR2010]. In the equilibrium states, some long-range interacting systems show the negative specific heat in the microcanonical ensemble [LW1968, HT1971] and the ensemble inequivalence between the micro canonical statistics and canonical statistics [BMR2001]. They are brought about by the lack of additivity [CDR2009].

In the non-equilibrium dynamics, one remarkable phenomenon is that a long-range interaction system is likely to be trapped in quasi-stationary states (QSSs), and accordingly a very long time is needed to reach the thermal equilibrium state. The duration of those QSSs increases according to the system size, and diverges if one takes the thermodynamic limit [BT2008, YBB+2004, BBD+2006, Cha2010, dBMR2011, TFL2011, Cha2012]. It is a widely accepted understanding that the equilibration is brought about by the finite size effect.

A way to analyze a Hamiltonian system with long-range interaction is to use the Vlasov equation or the collisionless Boltzmann equation [Ich1973, LP1981, BT2008], which can be derived by taking the limit $N \rightarrow \infty$ where N is the number of elements [BH1977, Dob1979, Spo1991]. The QSSs are recognized to be associated with stable stationary solutions to the Vlasov equation, and all the results exhibited in this thesis are based on this equation.

The latter part of this chapter is organized as follows. We first introduce systems with long-range interaction in Section 1.1. The Vlasov equation is derived from the N -body dynamical system in Section 1.2. Section 1.3 contains a brief review of QSSs and relaxation process. Section 1.4 is devoted to show the outline of this thesis.

1.1 Systems with long-range interaction

Let us consider an N -body system in \mathbb{R}^d with the Hamiltonian

$$H_N = \sum_{i=1}^N \frac{p_i^2}{2} + \frac{1}{2} \sum_{i \neq j}^N V(q_i - q_j) + \sum_{i=1}^N U(q_i), \quad (1.1)$$

$$q_i \in \mathbb{R}^d, \quad p_i \in \mathbb{R}^d, \quad i = 1, 2, \dots, N,$$

where V and U are inter-particle and onsite potentials respectively. When asymptotic behavior of the potential term $V(q)$ as $q \rightarrow \infty$ is given by

$$V(q) \sim |q|^{-\alpha}, \quad \alpha \leq d, \quad (1.2)$$

the system (1.1) is called the long-range interacting system. It is shown that the extensivity of the energy breaks if and only if $\alpha \leq d$, and so does the additivity when $\alpha \leq d$. Let us see it after Ref. [CDR2009] by estimating the total energy E_{tot} of the system whose inter-particle potential $V(q)$ is bounded and is asymptotically $V(q) \sim |q|^{-\alpha}$. For simplicity, we assume that the particles are distributed uniformly in the d -dimensional ball B_R of radius R . The potential energy ϵ_{cent} of the particle on the center of the ball is estimated as

$$\begin{aligned} \epsilon_{\text{cent}} &= \int_{B_R} V(q) dq^d \sim \int_0^R V(r) r^{d-1} dr \\ &\sim \begin{cases} \ln R + C, & \alpha = d, \\ R^{d-\alpha} + C, & \alpha \neq d, \end{cases} \end{aligned} \quad (1.3)$$

where C is a constant. Let V_R be the volume of the ball B_R . The total energy $E_{\text{tot}} \sim V_R \epsilon_{\text{cent}}$ can be estimated as follows

$$E_{\text{tot}} \sim \begin{cases} \frac{1}{d} V_R \ln V_R + C V_R, & \alpha = d, \\ V_R^{2-\alpha/d} + C V_R, & \alpha \neq d, \end{cases} \quad (1.4)$$

where we have used a scaling relation $V_R \propto R^{1/d}$. The asymptotic behavior of E_{tot} as $V_R \rightarrow \infty$ is

$$E_{\text{tot}} \sim \begin{cases} V_R, & \alpha > d, \\ V_R \ln V_R, & \alpha = d, \\ V_R^{2-\alpha/d}, & \alpha < d, \end{cases} \quad (1.5)$$

and it results in that E_{tot} is not extensive if and only if $\alpha \leq d$.

The gravitational interaction ($\alpha = 1, d = 3$), the Coulomb interaction ($\alpha = 1, d = 3$), the dipole interaction ($\alpha = 3, d = 3$), and the 2D point-vortex interaction ($V(q) \sim \ln |q|$ and $\alpha = 0, d = 2$) are well known long-range interaction.

Extensive systems We are interested in the macroscopic property of the systems with long-range interaction. Then, we are to focus on the models without additivity but with extensivity, so that we are able to look into the equilibrium and non-equilibrium statistical physics and dynamics of the systems with long-range interaction in the thermodynamic limit $N \rightarrow \infty$. We can give the extensivity by putting the factor $1/N$ to the inter-particle potential as

$$H_N = \sum_{i=1}^N \frac{p_i^2}{2} + \frac{1}{2N} \sum_{i \neq j}^N V(q_i - q_j) + \sum_{i=1}^N U(q_i), \quad (1.6)$$

$$q_i \in \Lambda \subset \mathbb{R}^d, \quad p_i \in \mathbb{R}^d, \quad i = 1, 2, \dots, N,$$

where Λ is a d -dimensional connected subset of \mathbb{R}^d , and we assume that V and U have no singularity and that V is an even function. In this thesis we set d as 1.

1.2 Vlasov equation

When the particle number N is large, dynamics of the Hamiltonian system (1.6) is shown to be well described with the single-body distribution f which is a solution to the Vlasov equation (or collisionless Boltzmann equation),

$$\frac{\partial f}{\partial t} + \{\mathcal{H}[f], f\} = 0, \quad (1.7)$$

where $\mathcal{H}[f]$ is the effective Hamiltonian

$$\begin{aligned} \mathcal{H}[f](q, p, t) &= \frac{p^2}{2} + \mathcal{V}[f](q, t) \\ \mathcal{V}[f](q, t) &= \int_{\Lambda} dq' \int_{-\infty}^{\infty} V(q - q') f(q', p', t) dp' + U(q), \end{aligned} \quad (1.8)$$

and the Poisson bracket $\{a, b\}$ is defined as

$$\{a, b\} = \frac{\partial a}{\partial p} \frac{\partial b}{\partial q} - \frac{\partial a}{\partial q} \frac{\partial b}{\partial p}. \quad (1.9)$$

This evolution equation had been used in the astrophysics by Jeans [Jea1915] around a century ago. Around 20 years later from Jeans' work, Vlasov [Vla1938] found this equation coupled with the Poisson equation or the Maxwell equation in the plasmas physics, and this equation has been called the Vlasov equation in the plasma physics. This equation is also called the collisionless Boltzmann equation in the astrophysics [BT2008], but there is another collisionless Boltzmann equation which describes short-time scale behavior of systems with short-range interaction [BGM2010]. We then call the equation (1.7) the Vlasov equation in this thesis to avoid confusion.

The Vlasov equation is derived from the Klimontovich equation [YBB+2004, CDR2009],

$$\begin{aligned} \frac{\partial \mu_t^N}{\partial t} + \sum_{i=1}^N p_i \frac{\partial \mu_t^N}{\partial q} - \sum_{i=1}^N \frac{\partial \Phi}{\partial q_i} \frac{\partial \mu_t^N}{\partial p} &= 0, \\ \Phi(q_1, \dots, q_N) &= \frac{1}{N} \sum_{i \neq j}^N V(q_i - q_j) + \sum_{i=1}^N U(q_i), \end{aligned} \quad (1.10)$$

which describes evolution of an empirical measure

$$\mu_t^N(q, p) dq dp \equiv \frac{1}{N} \sum_{i=1}^N \delta(q - q_i(t)) \delta(p - p_i(t)) dq dp, \quad (1.11)$$

where $(q_i(t), p_i(t))_{i=1}^N$ is a solution to the canonical equation of motion [BH1977, Dob1979, Spo1991]. The Klimontovich equation is obviously equivalent to the canonical equation of motion induced by the Hamiltonian (1.6). Braun and Hepp [BH1977] have rigorously shown that this discrete distribution (1.11) weakly converges to the single-body distribution $f(q, p, t) dq dp$ as $N \rightarrow \infty$ in any finite time scale and f is a solution to the Vlasov equation when $\mu_0^N(q, p) dq dp$ weakly converges to $f(q, p, 0) dq dp$ at initial. We exhibit more intuitive derivation of the Vlasov equation based on the Bogoliubov-Born-Green-Kirkwood-Yvon (BBGKY) hierarchy as Refs. [Ich1973, LP1981, Ina1996]. We start with the Liouville equation for the N -body density function $f_N(q_1, p_1, \dots, q_N, p_N)$,

$$\frac{\partial f_N}{\partial t} + \{H_N, f_N\}_N = 0, \quad (1.12)$$

where the Poisson bracket $\{a_N, b_N\}_N$ is defined as

$$\{a_N, b_N\}_N = \sum_{i=1}^N \left(\frac{\partial a_N}{\partial p_i} \frac{\partial b_N}{\partial q_i} - \frac{\partial a_N}{\partial q_i} \frac{\partial b_N}{\partial p_i} \right). \quad (1.13)$$

The reduced n -body distribution f_n is defined as

$$f_n(q_1, p_1, \dots, q_n, p_n) = \int \cdots \int f_N(q_1, p_1, \dots, q_N, p_N) \prod_{i=n+1}^N dq_i dp_i. \quad (1.14)$$

Integrating both sides of the Liouville equation (1.12) with respect to $\prod_{i=2}^N dq_i dp_i$, we obtain the equation

$$\frac{\partial f_1}{\partial t} + p \frac{\partial f_1}{\partial q} - \frac{\partial U}{\partial q} \frac{\partial f_1}{\partial p} - \iint \frac{\partial V(q - q')}{\partial q} \frac{\partial f_2}{\partial q}(q, p, q', p', t) dq' dp' = 0, \quad (1.15)$$

where we have approximated $(N - 1)/N \simeq 1$. We note that the equation (1.15) is not closed for f_1 . In order to make (1.15) closed, we here neglect the correlation between two elements, that is,

$$f_2(q, p, q', p', t) \simeq f_1(q, p, t) f_1(q', p', t). \quad (1.16)$$

This approximation means that we look on a system consisting of N interacting particles (1.6) as a system consisting of N independent particles moving in the mean-field according to the effective Hamiltonian (1.8), so that the approximation (1.16) is indeed the mean-field approximation. Substituting Eq. (1.16) into Eq. (1.15), we obtain the Vlasov equation (1.7) with the effective Hamiltonian (1.8).

1.3 Quasi-stationary states and relaxation process

The QSSs are recognized as stable stationary solutions to the Vlasov equation as we mentioned above, so that it may be reasonable to set our footing on the Vlasov equation (1.7) for the theoretical investigation for QSSs.

The relaxation process is schematically shown in Fig. 1.1. First, the system rapidly relaxes to a QSS associated with a stable stationary solution to the Vlasov equation. After a long time passes, the effect of the term which we have neglected in the mean-field approximation (1.16) becomes significant and non-negligible, and the system slowly relaxes to the equilibrium states due to the finite N effect [YBB+2004, BBD+2006]. The duration of QSSs is reported as $O(N^{1.7})$ for spatially homogeneous QSSs of the HMF model [YBB+2004], $O(N^{1.0})$ for spatially inhomogeneous QSSs [Cha2010, Cha2012, OPY2013], $O(N/\ln N)$ for stellar systems [BT2008], and $O(\ln N)$ for the α -HMF model with $\alpha = 1$ ($d = 1$) [TFL2011].

It should be noted that the QSSs dealt in this thesis are different from the meta-stable states, which can be observed in systems with both short- and long-range interaction, and described by using the Boltzmann-Gibbs statistics. A meta-stable equilibrium is said to be a local minimum of the free energy with some order parameters or local maximum of the entropy with those. These free energy and entropy are derived from Boltzmann-Gibbs statistics. In contrast, the QSS is described with non-Boltzmann-Gibbs statistics and this is one of the remarkable concepts in systems with long-range interaction. One of non-Boltzmann-Gibbs statistics is the Lynden-Bell statistics [Lyn1967] which is summarized in Appendix D.1. The QSSs are often thought to be realized as the global maximum of the non-Boltzmann-Gibbs entropy [Cha2006, AFB+2007], or thought to be dynamical concepts such as the core-halo structure [PL2011] or conservation of the single-body energy [dBMR2011].

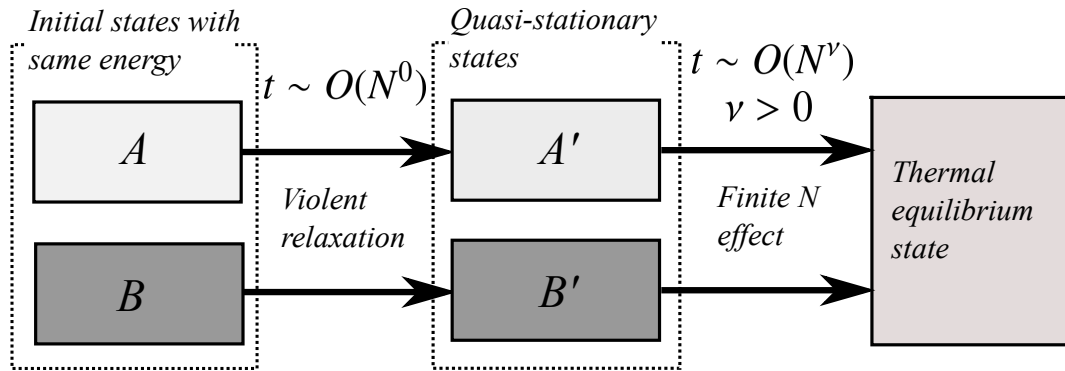


Figure 1.1: Schematic picture of the relaxation process: Two initial states A and B have the same value of energy density, but associated distributions are different from each other. The system rapidly relaxes to a QSS, and this process is called violent relaxation. One remarkable difference between QSSs and thermal equilibria is that QSSs depend on the parameter other than the invariant macroscopic quantities such as the energy density.

1.4 Outline of the thesis

Let us summarize the structure of this thesis in this section.

We are going to propose analytical procedures to explore non-equilibrium QSSs in this thesis. These procedures have already been used in or around the equilibrium state and we are to modify them by setting our footing on the Vlasov equation. Further, we are going to explore the critical phenomena in QSSs through using the Hamiltonian mean-field (HMF) model which is simple but has typical long-range features, by using the proposed procedures.

The HMF model, a frequently used toy model, is then introduced in Chapter 2 and we quickly review the statistical mechanics, the Vlasov equation and the linearized Vlasov equation for the HMF model. A useful tool to analyze perturbations around the spatially inhomogeneous solutions, such as the explicit forms of angle-action variables, dispersion functions or spectral functions are exhibited in this chapter. We also introduce the generalized HMF model there.

As we have mentioned, the QSSs are recognized to be associated with the stable stationary solutions to the Vlasov equation, and the Vlasov equation has infinitely many stationary solutions. The stability analysis is then considered to be a first step to look into the QSS, because we should determine whether the given stationary solution can be associated with the QSS or not. For spatially homogeneous solutions, the spectral and formal stability criteria have been already derived [YBB+2004, CD2009], and then, this fact means that the linear stability also has been explored [HMRW1985]. On the other hand, for spatially inhomogeneous solutions, explicit forms of stability criteria such as those for the spatially homogeneous solutions have not been found, although stability of spatially inhomogeneous stationary states has been investigated in the astrophysics context [BT2008]. In Chapter 3, stability of spatially inhomogeneous stationary solutions to the Vlasov equation is investigated for the HMF model to provide the spectral and the most refined formal stability criteria in the form of necessary and sufficient conditions [Oga2013]. These criteria determine stability of spatially inhomogeneous solutions, while a less refined formal stability criterion [CC2010] can not do. It is shown that some of such solutions can be found in a family of stationary solutions to the Vlasov equation, which is parametrized with macroscopic quantities and has a two phase coexistence region in the parameter plane [AFRY2007]. The criteria are derived for the HMF model without external field, but we discuss application for the other systems at the end of this chapter.

We next look into the dynamics of perturbations induced by external force around the stable stationary solutions to the Vlasov equation. In the QSSs, operation with external force has not been focused on until recent studies [PGN2012, OY2012, Cha2013], although it is an important concept in the thermodynamics and it may be compatible with an experimental setting. The linear response theory based on the Vlasov equation is then proposed for spatially 1D systems with periodic boundary condition in Chapter 4 as a first step to construct the thermodynamics theory for QSSs. The proposed theory is applicable both to spatially homogeneous and to spatially inhomogeneous QSSs and is demonstrated in the HMF model. Both in the homogeneous and inhomogeneous cases, zero-field susceptibility is explicitly obtained. In the homogeneous case, Curie-Weiss like law is suggested in a high-energy region. On the other hand, in the inhomogeneous case, a scaling rule between two critical exponents is found, and this scaling rule is not derived in the equilibrium statistical mechanics. Further, as application of this linear response theory, we extract non-equilibrium dynamics in the unforced system by use of time-dependent oscillating external fields and the resonance absorption.

It should be emphasized that we look into the given stationary solutions to the Vlasov equation in Chapters 3 and 4. However, the Vlasov equation has infinitely many stationary solutions, and QSSs depend on not only conservative quantities such as the energy density but also the parameter other than the invariant macroscopic quantities, for example, the order parameter at initial non-stationary state. Determining QSSs with respect to given initial non-stationary states is still a hard problem and is investigated in Refs. [Cha2006, AFB+2007, AFRY2007, Yam2008, LPR2008, LPT2008, JW2011, PL2011, dBMR2011, PL2013] for example. The universal theory to solve this problem has not been found yet. We do not get involved with the problem itself in this thesis. Let us focus on the statistical procedure based on a non-Boltzmann-Gibbs entropy. Once we set our footing on a non-Boltzmann-Gibbs entropy, we are allowed to discuss the non-equilibrium phase transition in QSSs based on it. The non-equilibrium phase transition of the HMF model in QSSs is investigated in Chapter 5. Existence of the non-equilibrium tricritical point has been revealed in the HMF model [AFRY2007] by a non-equilibrium statistical mechanics pioneered by Lynden-Bell [Lyn1967]. This statistical mechanics gives a distribution function containing unknown parameters, and parameters are determined by solving simultaneous equations depending on a given non-stationary initial state. Due to difficulty in solving these equations, pointwise numerical detection of the tricritical point has been unavoidable on a plane characterizing a family of initial non-stationary states. In order to look into the tricritical point, we expand the simultaneous equations with respect to the order parameter and reduce them to one algebraic equation. The tricritical point is precisely identified by analyzing coefficients of the reduced equation.

Chapter 6 is devoted to a conclusion and perspective.

Chapter 2

Hamiltonian mean-field model

In the last chapter, we have made a brief review of the dynamics and statistical physics for systems with long-range interaction. In practice, we often use simple toy models to investigate the long-range features of many body systems theoretically. The HMF model is a simple toy model which shows typical long-range features. For instance, the HMF model has been used for investigating the non-equilibrium phase transitions [Cha2006, AFRY2007, SCDF2009, SCD2011, OY2011], the core-halo structure [PL2011], the creation of small traveling clusters [BY2009], the construction of traveling clusters [Yam2011], and the relaxation process with long-range interaction, which has been reviewed in Section 1.3 after Refs. [YBB+2004, BBD+2006]. The HMF model especially makes it possible to investigate dynamics around specially inhomogeneous QSSs [BOY2010, BOY2011, OY2012]. Further, this model is closely related to a model for the collective atomic recoil laser [BS1994]. This chapter is organized as follows. We first exhibit the definition and interpretations of the HMF model in Section 2.1. We summarize the canonical equilibrium state in Section 2.2. In Section 2.3, we introduce the Vlasov equation for the HMF model. We look into the dynamics of perturbations around the stationary states with the linearized Vlasov equation in Section 2.4. In Section 2.5, we introduce the generalized HMF model.

2.1 Hamiltonian mean-field model

In this section, we introduce the HMF model. The Hamiltonian of the HMF model is as follows:

$$H_N = \sum_{i=1}^N \frac{p_i^2}{2} + \frac{1}{2N} \sum_{i,j=1}^N (1 - \cos(q_i - q_j)) - h_x \sum_{i=1}^N \cos q_i - h_y \sum_{i=1}^N \sin q_i, \quad (2.1)$$
$$p_i \in \mathbb{R}, \quad q_i \in [-\pi, \pi), \quad i = 1, 2, \dots, N,$$

where the periodic boundary condition is asserted for each q_i . We often look into the dynamics of the HMF model through observing the vector

$$\vec{M}_N \equiv (M_x^N, M_y^N)^T = \frac{1}{N} \sum_{i=1}^N (\cos q_i, \sin q_i)^T, \quad (2.2)$$

where the symbol T represents transposing. The vector \vec{M}_N is called an order parameter or the “magnetization” vector. Thanks to the translational symmetry, we can choose the direction of the external field $\vec{h} = (h_x, h_y)^T$ so that $\vec{h} = (h, 0)^T$ without loss of generality. Then, we rewrite the Hamiltonian (2.1) as

$$H_N = \sum_{i=1}^N \frac{p_i^2}{2} + \frac{1}{2N} \sum_{i,j=1}^N (1 - \cos(q_i - q_j)) - h \sum_{i=1}^N \cos q_i, \quad (2.3)$$

$$p_i \in \mathbb{R}, \quad q_i \in [-\pi, \pi), \quad i = 1, 2, \dots, N.$$

This model can be interpreted in two ways as follows:

- The HMF model can be looked on as a ferromagnetic model with all-to-all interaction, where we look on $(\cos q_i, \sin q_i)^T$ and h as an internal degree of freedom such as “XY-spin” on the i -th lattice point r_i and the external magnetic field, respectively. This picture makes it possible to clearly understand why the HMF model is a simple long-range interaction system. In this picture, the order parameter (2.2) is looked on as a “magnetization” vector as in the spin system. This picture is illustrated in Fig. 2.1(a).
- On the other hand, this model can be looked on as a dynamical systems with N unit mass particles moving on the circle S^1 , or a simplified gravitational model [IK1993, Ina1993, Ina1996]. In this picture, the order parameter (2.2) is thought to represent how the particles collect on the circle S^1 . This picture is illustrated in Fig. 2.1(b).

From the former view, the HMF model is generalized to the model whose site-site interaction is not uniform and is long-range. This generalized model makes it possible for us to look into the dynamics of long-range but not mean-field interaction systems with the same analytical procedure for the HMF model. We will see that in Section 2.5.

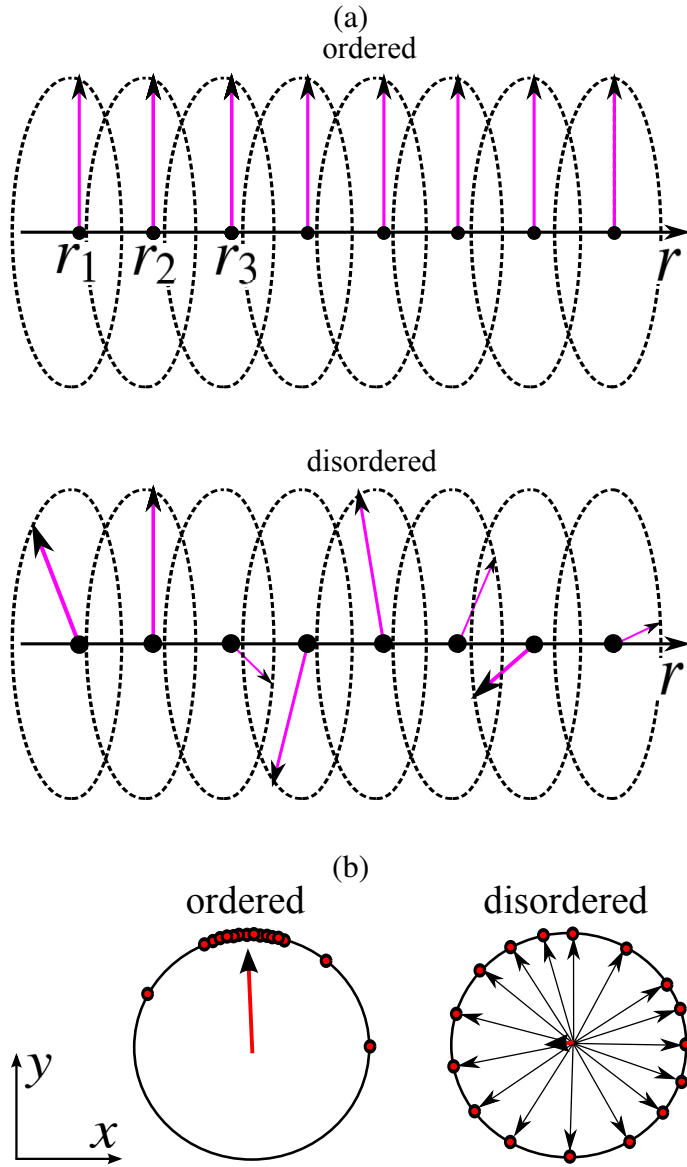


Figure 2.1: Two kinds of interpretation of the HMF model. The HMF model is looked on as an infinite-range XY-spin model on the one-dimensional lattice in the panel (a). The panel (b) shows that the HMF model can be looked on as the dynamical system consisting of moving particles on the circle S^1 . The red arrows describe the order parameters.

2.2 Statistical mechanics

The partition function of the N -body HMF model with the temperature $T = \beta^{-1}$ in the external field $\vec{h} = (h, 0)$ is computed as follows:

$$\begin{aligned}
Z(\beta, h, N) &= \int \cdots \int \exp \left[-\beta \left(H_N - h \sum_{i=1}^N \cos q_i \right) \right] \prod_{i=1}^N dq_i dp_i \\
&= \left(\frac{2\pi e^{-\beta}}{\beta} \right)^{N/2} \int \cdots \int \exp \left(\frac{\beta}{2N} \left[\left(\sum_{i=1}^N \cos q_i \right)^2 + \left(\sum_{i=1}^N \sin q_i \right)^2 \right] + \beta h \sum_{i=1}^N \cos q_i \right) dq_1 \cdots dq_N \quad (2.4) \\
&= \left(\frac{2\pi e^{-\beta}}{\beta} \right)^{N/2} \int \cdots \int \exp \left(\frac{N\beta}{2} (M_x^{N2} + M_y^{N2} + 2hM_x^N) \right) dq_1 \cdots dq_N,
\end{aligned}$$

where we have used Eq. (2.2). To decompose this integral with respect to $\prod_{i=1}^N dq_i$ into independent N integrals with respect to dq_i ($i = 1, 2, \dots, N$), we use the Hubbard-Stratonovich transformation [CDR2009, NO2011],

$$e^{ay^2} = \sqrt{\frac{a}{\pi}} \int_{-\infty}^{\infty} e^{-ax^2 + 2axy} dx, \quad a > 0. \quad (2.5)$$

The integral in Eq. (2.4) is then arranged as

$$\begin{aligned}
Z(\beta, h, N) &= \left(\frac{2\pi e^{-\beta}}{\beta} \right)^{N/2} \frac{N\beta}{2\pi} \int \cdots \int dq_1 \cdots dq_N \int_{-\infty}^{\infty} e^{-\frac{N\beta}{2}(m_x^2 - 2(m_x + h)M_x^N)} dm_x \int_{-\infty}^{\infty} e^{-\frac{N\beta}{2}(m_y^2 - 2m_y M_y^N)} dm_y \\
&= \left(\frac{2\pi e^{-\beta}}{\beta} \right)^{N/2} \frac{N\beta}{2\pi} \iint_{\mathbb{R}^2} dm_x dm_y e^{-N\beta(m_x^2 + m_y^2)/2} \\
&\quad \times \int \cdots \int \exp \left(\beta \left[(m_x + h) \sum_{i=1}^N \cos q_i + m_y \sum_{i=1}^N \sin q_i \right] \right) dq_1 \cdots dq_N \\
&= \left(\frac{2\pi e^{-\beta}}{\beta} \right)^{N/2} \frac{N\beta}{2\pi} \iint_{\mathbb{R}^2} dm_x dm_y \exp \left(-N \left[\frac{\beta}{2} (m_x^2 + m_y^2) - \ln \left(2\pi I_0 \left(\beta \sqrt{(m_x + h)^2 + m_y^2} \right) \right) \right] \right), \quad (2.6)
\end{aligned}$$

where we have shifted q_i with $q_i \mapsto q_i + \tan^{-1}(m_y/(m_x + h))$, and where I_n is the modified Bessel function of order n [AS1972] given by

$$I_n(z) \equiv \frac{1}{\pi} \int_0^\pi \cos(nq) e^{z \cos q} dq. \quad (2.7)$$

In the thermodynamic limit $N \rightarrow \infty$, we are able to compute integral in Eq. (2.6) using the saddle point method, so that we can obtain the free-energy density. We then seek a critical point of a function,

$$\phi(m_x, m_y) \equiv \frac{\beta}{2} (m_x^2 + m_y^2) - \ln I_0 \left(\beta \sqrt{(m_x + h)^2 + m_y^2} \right). \quad (2.8)$$

The dominant values of m_x and m_y of the integration in Eq. (2.6) satisfy the extremum condition

$$\frac{\partial \phi}{\partial m_i}(m_x, m_y) = 0, \quad i = x, y. \quad (2.9)$$

The condition (2.9) is written out as

$$\begin{aligned} m_x &= \frac{m_x + h}{\sqrt{(m_x + h)^2 + m_y^2}} \frac{I_1 \left(\beta \sqrt{(m_x + h)^2 + m_y^2} \right)}{I_0 \left(\beta \sqrt{(m_x + h)^2 + m_y^2} \right)}, \\ m_y &= \frac{m_y}{\sqrt{(m_x + h)^2 + m_y^2}} \frac{I_1 \left(\beta \sqrt{(m_x + h)^2 + m_y^2} \right)}{I_0 \left(\beta \sqrt{(m_x + h)^2 + m_y^2} \right)}. \end{aligned} \quad (2.10)$$

When $h > 0$, it is shown that $m_y = 0$, and Eq. (2.10) is simplified as

$$m_x = \frac{I_1(\beta(m_x + h))}{I_0(\beta(m_x + h))}. \quad (2.11)$$

When $h = 0$, the HMF model has rotational symmetry and we can choose the x direction so that $m_x \geq 0$ and $m_y = 0$. Then, the extremum condition (2.10) can be reduced as

$$m_x = \frac{I_1(\beta m_x)}{I_0(\beta m_x)}. \quad (2.12)$$

Let m_x^* be a solution to Eqs. (2.11) or (2.12). We can look on m_x^* as the order parameter or the magnetization, since the extremum condition for the second line of Eq. (2.6) is shown to be [NO2011]

$$m_x^* = \frac{1}{N} \sum_{i=1}^N \cos q_i = M_x^N \rightarrow M, \quad (N \rightarrow \infty). \quad (2.13)$$

The magnetization M is then plotted in Fig. 2.2 by solving Eq. (2.12). The second-order phase transition occurs at the critical temperature $T_c = 1/2$. The zero-field susceptibility χ is computed from Eq. (2.11) as

$$\chi = \left. \frac{\partial M}{\partial h} \right|_{h=0} = \begin{cases} \frac{T_c}{T - T_c}, & T > T_c, \\ \frac{1 - M^2 - T}{2[T - T_c(1 - M^2)]}, & T < T_c, \end{cases} \quad (2.14)$$

and is plotted in Fig. 2.2. In the vicinity of the critical point, M and χ are believed to behave as follows [NO2011]

$$\begin{aligned} M &\sim |T - T_c|^\beta, \quad T \lesssim T_c, \\ \chi &\sim \begin{cases} |T - T_c|^{-\gamma_+}, & T \gtrsim T_c, \\ |T - T_c|^{-\gamma_-}, & T \lesssim T_c. \end{cases} \end{aligned} \quad (2.15)$$

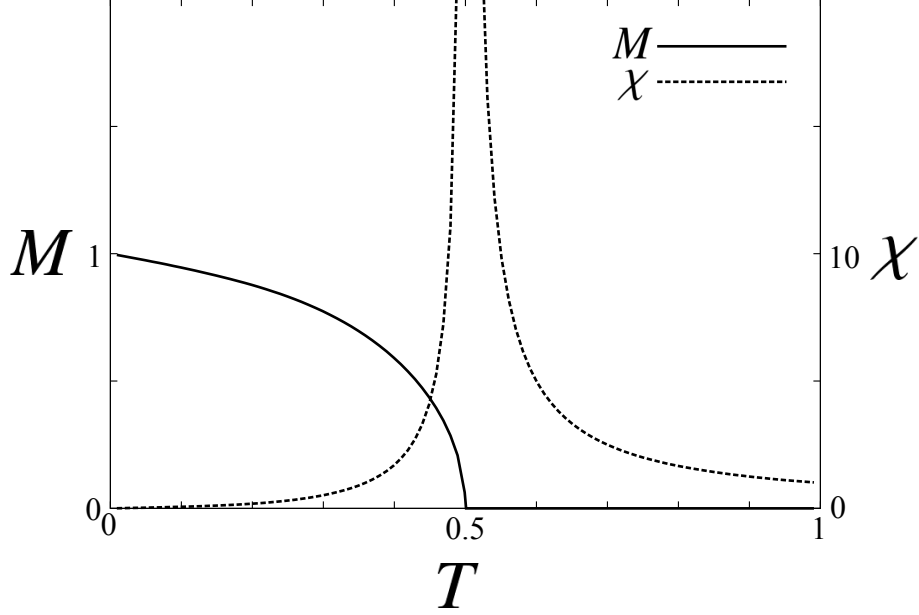


Figure 2.2: The order parameter (magnetization) M and the zero-field susceptibility χ are plotted as functions of the temperature T . The second-order phase transition occurs at the critical temperature $T_c = 1/2$.

The exponent β in this scaling law is not the inverse temperature. These critical exponents β and γ_{\pm} for the HMF model are $\beta = 1/2$ [AR1995] and $\gamma_{\pm} = 1$ [Cha2012], and they are in the mean-field universality class [NO2011].

2.3 Vlasov equation

As we mentioned in Section 1.2, in the limit of N tending to infinity, the time evolution of the HMF model can be well described in terms of the single-body distribution f on the μ space which coincides with $S^1 \times \mathbb{R}$ [BH1977, Dob1979, Spo1991]. The single-body distribution f is known to evolve according to the Vlasov equation,

$$\frac{\partial f}{\partial t} + \{\mathcal{H}[f], f\} = 0, \quad (2.16)$$

where $\mathcal{H}[f]$ is the effective single-body Hamiltonian defined to be

$$\begin{aligned} \mathcal{H}[f] &= \frac{p^2}{2} + \mathcal{V}[f](q, t), \\ \mathcal{V}[f] &= - \int_{-\pi}^{\pi} dq' \cos(q - q') \int_{-\infty}^{\infty} f(q', p', t) dp' - h \cos q, \\ p &\in \mathbb{R}, \quad q \in [-\pi, \pi). \end{aligned} \quad (2.17)$$

By averaging the distribution f with cosine and sine weights, the order parameter $\vec{M}[f] = (M_x[f], M_y[f])^T$ is defined to be

$$\begin{aligned} M_x[f](t) &= \iint_{\mu} \cos q f(q, p, t) dq dp, \\ M_y[f](t) &= \iint_{\mu} \sin q f(q, p, t) dq dp, \end{aligned} \quad (2.18)$$

where the symbol μ denotes the whole μ space, $S^1 \times \mathbb{R}$. This order parameter (2.18) is a continuous limit ($N \rightarrow \infty$) of the order parameter (2.2). We often perform theoretical analysis by using the continuous one (2.18), and check its results with the N -body simulations by use of the discrete one (2.2).

We remark on invariants under the Vlasov dynamics. In the Vlasov dynamics, the normalization condition

$$\mathcal{N}[f] \equiv \iint_{\mu} f(q, p, t) dq dp = 1, \quad (2.19)$$

is satisfied, and the momentum density

$$\mathcal{P}[f] \equiv \iint_{\mu} p f(q, p, t) dq dp, \quad (2.20)$$

and the energy density

$$\mathcal{U}[f] \equiv \iint_{\mu} \frac{p^2}{2} f(q, p, t) dq dp - \frac{1}{2} (M_x[f]^2 + M_y[f]^2) - h M_x[f], \quad (2.21)$$

are conserved. Additionally, a value of a functional

$$\mathcal{Q}[f] = \iint_{\mu} Q(f(q, p, t)) dq dp \quad (2.22)$$

is conserved in the Vlasov dynamics for any function Q , and such a functional is called a Casimir invariant. Those invariants are of importance in stability analysis and a non-equilibrium statistical mechanics based on the Vlasov equation.

2.4 Linearized Vlasov equation

The linearized Vlasov equation is a useful tool for looking into dynamics around QSSs. Let f_0 denote a stationary solution to the Vlasov equation, and depend on (q, p) only through the effective single-body Hamiltonian $\mathcal{H}[f_0] = p^2/2 - (M_0 + h) \cos q$. Then, a small perturbation f_1 around f_0 is shown to obey, in some timescale, the linearized Vlasov equation

$$\begin{aligned} \frac{\partial f_1}{\partial t} &= \widehat{\mathcal{L}} f_1, \\ \widehat{\mathcal{L}} f_1 &:= -\{\mathcal{H}[f_0], f_1\} - \{\mathcal{V}[f_1], f_0\}. \end{aligned} \quad (2.23)$$

This equation can be analyzed by means of the Fourier-Laplace transformation. For the sake of physical interpretation, we define the Laplace transform of a function $g(t)$ to be

$$\tilde{g}(\omega) = \int_0^\infty g(t)e^{i\omega t} dt, \quad (2.24)$$

where $\text{Im}\omega > 0$ so that the integral converges. Through the Fourier series expansions with respect to q and the Laplace transformation with respect to t , Eq. (2.23) is brought into the dispersion relation $D(\omega) = 0$ [Lan1946, LP1981, Cha2007, BOY2010]. A nontrivial mode $\sim e^{-i\omega t}$ arises when $D(\omega) = 0$. The explicit form of the dispersion relations for spatially homogeneous stationary states and for spatially inhomogeneous stationary states will be derived in Sections 2.4.1 and 2.4.2 respectively. We call $D(\omega)$ a dispersion function, which is said to be a dielectric function in the context of the plasmas physics. A root ω of this dispersion relation with positive imaginary part is in one-to-one correspondence with the eigenvalue $-i\omega$ of the linear operator $\widehat{\mathcal{L}}$. The detail of this fact will be reviewed in Sections 2.4.1 and 2.4.2.

The domain of the dispersion function $D(\omega)$ is the upper half ω plane, but it can be analytically continued to the lower half ω plane [Lan1946, LP1981]. A root of the dispersion relation on the lower half plane causes the exponential damping of the order parameter for the small perturbation $\vec{M}[f_1] = (M_x[f_1], M_y[f_1])^T$, which is called the Landau damping [Lan1946, LP1981]. Such a root is not an eigenvalue, but is called a resonance pole, a Landau pole [BOY2010], or a fake eigenvalue [SMM1992].

We remark on embedded eigenvalues of the linear operator $\widehat{\mathcal{L}}$ on the imaginary axis. The linear operator $\widehat{\mathcal{L}}$ may have continuous spectra lying on the imaginary axis [CH1989]. An “eigenvalue” with zero real part is occasionally embedded in the continuous spectra and such an “eigenvalue” is called an embedded eigenvalue.

In the latter part of this section, the spectral function $\Lambda(\omega)$ and the dispersion relation are derived for both homogeneous and inhomogeneous stationary states. The zero points of the spectral function determine eigenvalues of the linearized Vlasov operator (2.23). We review the relation between eigenvalues of the linearized Vlasov operator (2.23) and roots of the dispersion relation after Refs. [vaK1955, Cas1959, CH1989].

2.4.1 Spectral function and dispersion relation in spatially homogeneous stationary state

We first deal with a spatially homogeneous stationary solution, and then, we set the external field $h = 0$. Let $f_0(p)$ be a spatially homogeneous, even, unimodal, and smooth function. Let $\widehat{\mathcal{L}}$ be the associated linearized Vlasov operator which is defined by Eq. (2.23). Then, the linearized Vlasov equation around $f_0(p)$ takes the form

$$\frac{\partial f_1}{\partial t} + p \frac{\partial f_1}{\partial q} - f'_0(p) \frac{\partial}{\partial q} \mathcal{V}[f_1] = 0. \quad (2.25)$$

We expand the both sides of Eq. (2.25) into the Fourier series to find that the amplitude of the k -th Fourier mode $f_{1,k}(p, t)$ obeys one of the following equations

$$\frac{\partial f_{1,k}}{\partial t} = \begin{cases} -ik \left[p f_{1,k}(p, t) + \pi \int_{-\infty}^{\infty} f_{1,k}(p', t) dp' f'_0(p) \right], & |k| = 1, \\ -ik p f_{1,k}(p, t), & |k| \neq 1. \end{cases} \quad (2.26)$$

Spectral function For $|k| \neq 1$, there is no growth or damping modes. For $|k| = 1$, if λ is an eigenvalue of the linearized Vlasov operator $\widehat{\mathcal{L}}$, the associated eigenfunction can be written as $\tilde{f}_{1,k}^\lambda(p) e^{\lambda t}$, and we get the equation for $\tilde{f}_{1,k}^\lambda(p)$:

$$\tilde{f}_{1,k}^\lambda(p) = -\frac{\pi f'_0(p)}{p - i\lambda/k} \int_{-\infty}^{\infty} \tilde{f}_{1,k}^\lambda(p') dp'. \quad (2.27)$$

Integrating this equation over the whole \mathbb{R} results in

$$\int_{-\infty}^{\infty} \tilde{f}_{1,k}^\lambda(p') dp' \left[1 + \pi \int_{-\infty}^{\infty} \frac{f'_0(p)}{p - i\lambda/k} dp \right] = 0, \quad (2.28)$$

which is rewritten as

$$\Lambda(i\lambda/k) \int_{-\infty}^{\infty} \tilde{f}_{1,k}^\lambda(p') dp' = 0, \quad (2.29)$$

where Λ is defined to be

$$\Lambda(\omega) = 1 + \pi \int_{-\infty}^{\infty} \frac{f'_0(p)}{p - \omega} dp, \quad (2.30)$$

and is called the spectral function defined on $\mathbb{C} \setminus \mathbb{R}$. If the factor including $\tilde{f}_{1,k}$ in Eq. (2.28) vanishes, that is, if

$$\int_{-\infty}^{\infty} \tilde{f}_{1,k}^\lambda(p') dp' = 0, \quad (2.31)$$

then $\tilde{f}_{1,k}(p)$ vanishes owing to Eq. (2.27). It then, follows from Eq. (2.29) that if λ is an eigenvalue of the linearized Vlasov operator $\widehat{\mathcal{L}}$, the equation $\Lambda(i\lambda/k) = 0$ should be satisfied for $k = 1$ or for $k = -1$. It is to be remarked that if the stationary solution f_0 is even unimodal smooth function, the associated spectral function satisfies the relation,

$$\Lambda(\omega) = \Lambda(-\omega) = \Lambda(\omega^*)^* = \Lambda(-\omega^*)^*, \quad (2.32)$$

where z^* denotes a complex conjugate of $z \in \mathbb{C}$.

Dispersion relation We next consider the initial value problem (2.25) with an initial condition $f_1(q, p, 0) = g(q, p)$, i.e., $f_{1,k}(p, 0) = g_k(p)$ for $k \in \mathbb{Z}$. Taking the Laplace transformation of the both sides of Eq. (2.26), we get the equation

$$\tilde{f}_{1,k}(p, \omega) - \pi \frac{f'_0(p)}{p - \omega/k} \int_{-\infty}^{\infty} \tilde{f}_{1,k}(p', \omega) dp' = \frac{g_k(p)}{i(kp - \omega)} \quad (2.33)$$

for $k = \pm 1$. Integrating the both sides of Eq. (2.33) with respect to p over \mathbb{R} , we obtain

$$D(\omega/k) \int_{-\infty}^{\infty} \tilde{f}_{1,k}(p, \omega) dp = G_k(\omega) \quad (2.34)$$

where

$$D(\omega) = 1 + \pi \int_{-\infty}^{\infty} \frac{f'_0(p)}{p - \omega} dp, \quad (2.35)$$

and

$$G_k(\omega) \equiv \int_{-\infty}^{\infty} \frac{g_k(p)}{i(kp - \omega)} dp. \quad (2.36)$$

The dispersion function $D(\omega)$ and the function $G_k(\omega)$ are derived by use of the Laplace transformation, and hence, the domain of $D(\omega)$ and of $G_k(\omega)$ is the upper half ω plane. The domain is extended as follows [Lan1946]

$$D(\omega) = \begin{cases} 1 + \pi \int_{-\infty}^{\infty} \frac{f'_0(p)}{p - \omega} dp, & \text{Im}\omega > 0, \\ 1 + \pi \text{P.V.} \int_{-\infty}^{\infty} \frac{f'_0(p)}{p - \omega} dp + i\pi^2 f'_0(\omega) & \text{Im}\omega = 0, \\ 1 + \pi \int_{-\infty}^{\infty} \frac{f'_0(p)}{p - \omega} dp + 2i\pi^2 f'_0(\omega) & \text{Im}\omega < 0, \end{cases} \quad (2.37)$$

by deforming a path of integration in Eq. (2.35) as illustrated in Fig. 2.3, where P.V. means taking a Cauchy principal value. By using the same procedure, the function $G_k(\omega)$ can be analytically continued to the whole \mathbb{C} .

Taking the inverse Laplace transformation, we obtain

$$\frac{1}{2\pi} \iint_{\mu} e^{-ikq} f_1(p, q, t) dq dp = \frac{1}{2\pi} \int_{\Gamma} \frac{G_k(\omega)}{D(\omega/k)} e^{-i\omega t} d\omega, \quad k = \pm 1, \quad (2.38)$$

where Γ denotes the Bromwich path (see Fig. 2.4), the linear dynamics of the order parameter $(M_{1,x}(t), M_{1,y}(t))^T$ is clarified. The nontrivial mode $\sim e^{i\omega t}$ arises when the dispersion relation $D(\omega) = 0$ satisfies. We note that G_k has no branch point as long as $g_k(p)$ is smooth and the perturbation (2.38) is determined by only the roots of the dispersion relation.

Here we note that the relation between $\Lambda(\omega)$ and $D(\omega)$ for $\omega \in \mathbb{C} \setminus \mathbb{R}$:

$$D(\omega) = \begin{cases} \Lambda(\omega), & \text{Im}\omega > 0, \\ \Lambda(\omega) + 2i\pi^2 f'_0(\omega), & \text{Im}\omega < 0. \end{cases} \quad (2.39)$$

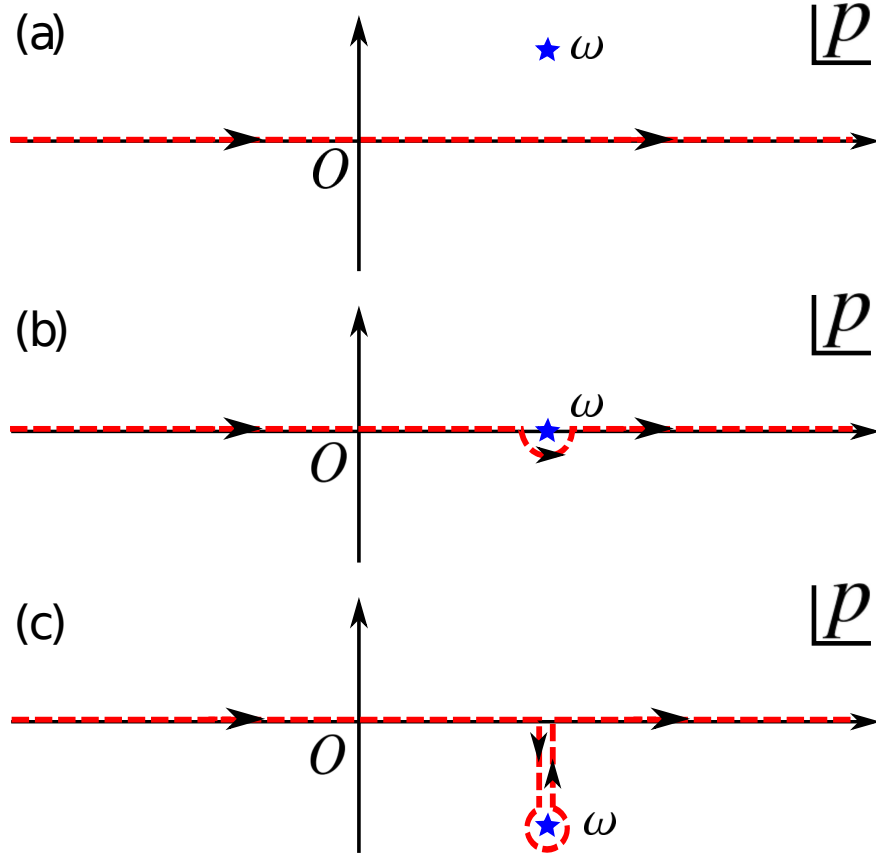


Figure 2.3: Illustration of the way to deforming the path of integration in Eq. (2.35). The red broken lines represent integration paths for each case: (a) $\text{Im}\omega > 0$, (b) $\text{Im}\omega = 0$, (c) $\text{Im}\omega < 0$.

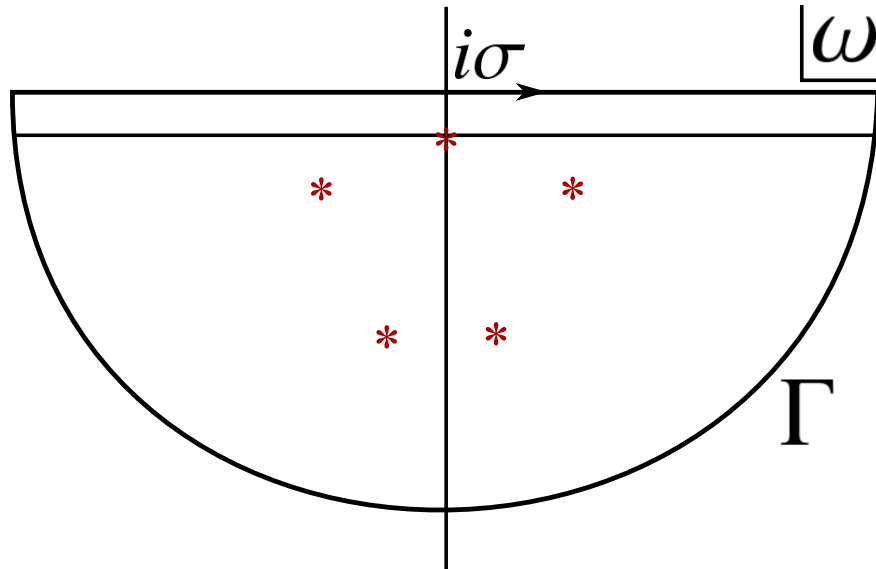


Figure 2.4: Schematic picture of the Bromwich path Γ . A red asterisk (*) denotes a root of the dispersion relation on the ω plane. The parameter σ is chosen so that all roots of the dispersion relation exist below the bold straight line, which runs from $-\infty + i\sigma$ to $\infty + i\sigma$.

2.4.2 Spectral function and dispersion relation in spatially inhomogeneous stationary state

So far, we have dealt with spatially homogeneous stationary solutions. The linearized Vlasov equation (2.23) around a spatially inhomogeneous stationary solution $f_0(q, p)$ takes the form

$$\frac{\partial f_1}{\partial t} + p \frac{\partial f_1}{\partial q} - \frac{\partial f_0}{\partial p} \frac{\partial}{\partial q} \mathcal{V}[f_1] - \frac{\partial f_1}{\partial p} \frac{\partial}{\partial q} \mathcal{V}[f_0] = 0. \quad (2.40)$$

The factor $\partial f_1 / \partial p$ prevents us deriving the spectral and dispersion functions, since this equation cannot be reduced to the algebraic equation by use of the Fourier-Laplace transformation. This problem can be removed by using the angle-action coordinates.

Angle-action coordinates We show the outline of the way to construct the angle-action variables. The detail of constructing the angle-action coordinates for the pendulum can be found in Refs. [BOY2010, Bri2011].

We consider the external field $h = 0$ and the stationary solution f_0 can be written in the form

$$f_0(q, p) = \hat{f}_0(\mathcal{E}(q, p)), \quad \mathcal{E}(q, p) = \frac{p^2}{2} - M_0 \cos q, \quad (2.41)$$

where $M_0 = M_x[f_0]$. The following discussions can be applied to the case when $\vec{h} = (h, 0)^T \neq \vec{0}$ by replacing M_0 with $M_0 + h$. The effective single-body Hamiltonian $\mathcal{H}[f_0] = \mathcal{E}(q, p)$ is the same with the Hamiltonian of the pendulum.

To construct a bijective mapping of (q, p) to (θ, J) , we divide the μ space into three regions, U_1 , U_2 , and U_3 , which are defined, respectively, as

$$\begin{aligned} U_1 &= \{(q, p) \mid \mathcal{E}(q, p) > M_0, p > 0\}, \\ U_2 &= \{(q, p) \mid |\mathcal{E}(q, p)| < M_0\}, \\ U_3 &= \{(q, p) \mid \mathcal{E}(q, p) > M_0, p < 0\}. \end{aligned} \quad (2.42)$$

According to this division of the μ space, we prepare the sets V_1 , V_2 , and V_3 defined to be

$$\begin{aligned} V_1 &= \{(\theta_1, J_1) \mid \theta_1 \in [-\pi, \pi), J_1 > 4\sqrt{M_0/\pi}\}, \\ V_2 &= \{(\theta_2, J_2) \mid \theta_2 \in [-\pi, \pi), 0 < J_2 < 8\sqrt{M_0/\pi}\}, \\ V_3 &= \{(\theta_3, J_3) \mid \theta_3 \in [-\pi, \pi), J_3 > 4\sqrt{M_0/\pi}\}, \end{aligned} \quad (2.43)$$

respectively. Then, the maps $(q, p) \mapsto (\theta_i, J_i) : U_i \rightarrow V_i$, for $i = 1, 2, 3$, are bijective. We illustrate the angle-action variables in three regions U_1 , U_2 , and U_3 in Fig. 2.5.

We note that a set $U_1 \cup U_2 \cup U_3$ does not coincide with the full μ space, since the μ space is actually $U_1 \cup U_2 \cup U_3 \cup U_{\text{sep}} \cup \{(0, 0)\}$, where $U_{\text{sep}} = \{(q, p) \mid \mathcal{E}(q, p) = M_0\}$ is a separatrix. The sets U_{sep} and $\{(0, 0)\}$ are not important. This is because we use the angle-action coordinates to express the dispersion function and the spectral function in the latter part of this thesis, and the angle-action variables appear only as integral variables. We then do not have to mention more on the boundaries of U_i , since the sets U_{sep} and $\{(0, 0)\}$ are null sets.

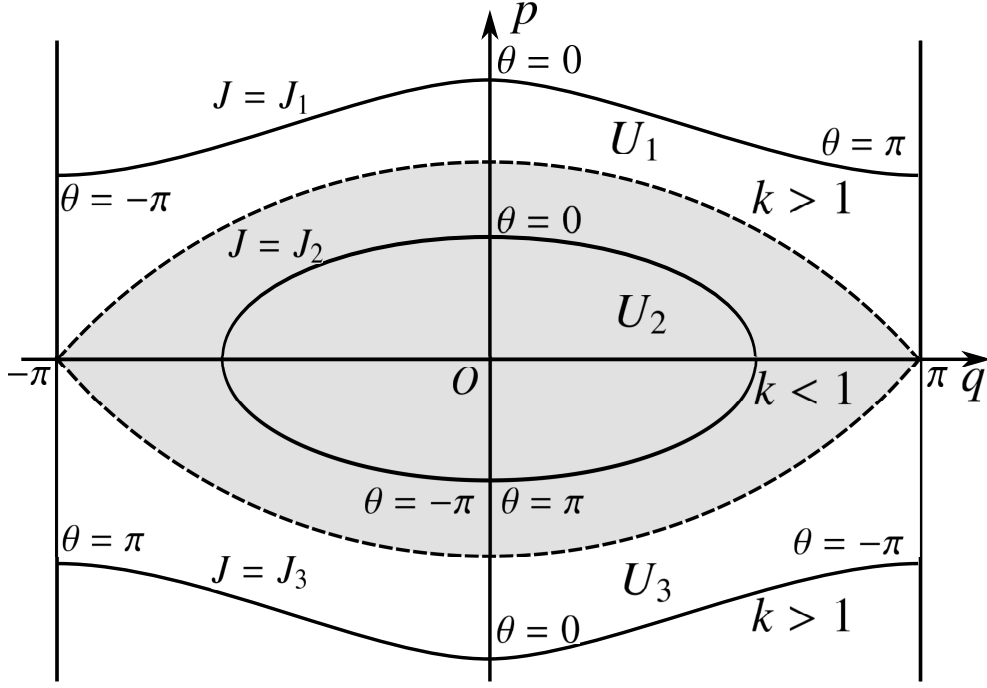


Figure 2.5: We illustrate the angle-action variables in regions U_i ($i = 1, 2, 3$) in the μ space. The broken curve is a separatrix. The region U_2 is the gray region surrounded by the separatrix. The solid curves in each regions are trajectories of the dynamics induced by the effective single-body Hamiltonian $\mathcal{H}[f_0](q, p) = \mathcal{E}(q, p) = p^2/2 - M_0 \cos q$.

For each region U_i , the angle-action variables (θ_i, J_i) are respectively introduced as follows [BOY2010, Bri2011]. The action variable J is given by

$$J = \frac{1}{2\pi} \oint p dq, \quad p = \pm \sqrt{2(\mathcal{E} - M_0 \cos q)}. \quad (2.44)$$

Then, each action variable J_i can be expressed as follows:

$$\begin{aligned} J_1 &= \frac{4\sqrt{M_0}}{\pi} k E(1/k), \quad (q, p) \in U_1, \\ J_2 &= \frac{8\sqrt{M_0}}{\pi} (E(k) - (1 - k^2)K(k)), \quad (q, p) \in U_2, \\ J_3 &= \frac{4\sqrt{M_0}}{\pi} k E(1/k), \quad (q, p) \in U_3, \end{aligned} \quad (2.45)$$

where the elliptic modulus k is given by

$$k = \sqrt{\frac{\mathcal{E} + M_0}{2M_0}}, \quad (2.46)$$

and where $K(k)$ and $E(k)$ are the first and the second kinds of complete elliptic integrals respectively [WW1927]. The definitions of them are summarized in Appendix A. We note that the

modulus k satisfies the relation

$$\begin{aligned}
k > 1 &\Leftrightarrow \mathcal{E} > M_0 \Leftrightarrow (q, p) \in U_1 \cup U_3, \\
k = 1 &\Leftrightarrow \mathcal{E} = M_0 \Leftrightarrow (q, p) \in U_{\text{sep}}, \\
0 < k < 1 &\Leftrightarrow |\mathcal{E}| < M_0 \Leftrightarrow (q, p) \in U_2, \\
k = 0 &\Leftrightarrow \mathcal{E} = -M_0 \Leftrightarrow (q, p) = (0, 0).
\end{aligned} \tag{2.47}$$

The angle variable θ is given by the generator function $W(q, J)$ of the canonical transformation $(q, p) \mapsto (\theta, J)$ as follows:

$$\theta = \frac{\partial W}{\partial J}(q, J), \quad W(q, J) = \int^q p(q', J) dq'. \tag{2.48}$$

The angle variables θ_i ($i = 1, 2, 3$) then satisfy the relations:

$$\begin{aligned}
q_1(\theta_1, J_1) &= 2 \sin^{-1} \left(k \operatorname{sn} \left(\frac{K(1/k)}{\pi} \theta_1, \frac{1}{k} \right) \right), \quad (q, p) \in U_1, \\
q_2(\theta_2, J_2) &= 2 \sin^{-1} \left(k \operatorname{sn} \left(\frac{2K(k)}{\pi} \theta_2, k \right) \right), \quad (q, p) \in U_2, \\
q_3(\theta_3, J_3) &= -2 \sin^{-1} \left(k \operatorname{sn} \left(\frac{K(1/k)}{\pi} \theta_3, \frac{1}{k} \right) \right), \quad (q, p) \in U_3,
\end{aligned} \tag{2.49}$$

respectively, and the functions $\sin q(\theta, J)$ and $\cos q(\theta, J(k))$ are expressed as

$$\sin q(\theta, J(k)) = \begin{cases} 2 \operatorname{sn} \left(\frac{K(1/k)}{\pi} \theta, \frac{1}{k} \right) \operatorname{cn} \left(\frac{K(1/k)}{\pi} \theta, \frac{1}{k} \right), & k > 1, p > 0, \\ -2 \operatorname{sn} \left(\frac{K(1/k)}{\pi} \theta, \frac{1}{k} \right) \operatorname{cn} \left(\frac{K(1/k)}{\pi} \theta, \frac{1}{k} \right), & k > 1, p < 0, \\ 2k \operatorname{sn} \left(\frac{2K(k)}{\pi} \theta, k \right) \operatorname{dn} \left(\frac{2K(k)}{\pi} \theta, k \right), & k < 1. \end{cases} \tag{2.50}$$

$$\cos q(\theta, J(k)) = \begin{cases} 1 - 2 \operatorname{sn}^2 \left(\frac{K(1/k)}{\pi} \theta, \frac{1}{k} \right), & k > 1, \\ 1 - 2k^2 \operatorname{sn}^2 \left(\frac{2K(k)}{\pi} \theta, k \right), & k < 1, \end{cases} \tag{2.51}$$

respectively, where $\operatorname{sn}(u, k)$, $\operatorname{cn}(u, k)$, and $\operatorname{dn}(u, k)$ are the Jacobian elliptic functions [WW1927]. The definitions of the Jacobian elliptic functions are summarized in Appendix A. The frequency $\Omega(J) = d\mathcal{H}[f_0]/dJ$ is expressed as follows [BOY2010],

$$\Omega(J(k)) = \begin{cases} \frac{\pi k \sqrt{M_0}}{K(1/k)}, & k > 1, \\ \frac{\pi \sqrt{M_0}}{2K(k)}, & k < 1. \end{cases} \tag{2.52}$$

According to these bijections, a function g whose arguments are the angle-action variables (θ, J) is denoted by

$$g(\theta, J) = \begin{cases} g_1(\theta_1, J_1), & (\theta, J) \in V_1, \\ g_2(\theta_2, J_2), & (\theta, J) \in V_2, \\ g_3(\theta_3, J_3), & (\theta, J) \in V_3, \end{cases} \quad (2.53)$$

respectively. We will omit the subscript i if no confusion arises. For notational simplicity, we denote the integral of the function (2.53) over the whole μ space by the left-hand side of the following equation

$$\iint_{\mu} g(\theta, J) d\theta dJ \equiv \sum_{i=1,2,3} \iint_{V_i} g_i(\theta_i, J_i) d\theta_i dJ_i. \quad (2.54)$$

In a similar manner, the integration of a function $f(J)$ is put in the form,

$$\int_L f(J) dJ \equiv \int_{4\sqrt{M_0}/\pi}^{\infty} f_1(J_1) dJ_1 + \int_0^{8\sqrt{M_0}/\pi} f_2(J_2) dJ_2 + \int_{4\sqrt{M_0}/\pi}^{\infty} f_3(J_3) dJ_3. \quad (2.55)$$

In the latter part of this thesis, the monotonicity of a function $f(J)$ with respect to J means the monotonicity of functions $f_i(J_i)$ with respect to J_i for each $i = 1, 2, 3$, respectively.

Spectral function Use of the angle-action coordinates makes it possible to apply the procedure introduced in the homogeneous case for the inhomogeneous case. Let us rewrite the Poisson bracket as

$$\{a, b\} = \frac{\partial a}{\partial J} \frac{\partial b}{\partial \theta} - \frac{\partial a}{\partial \theta} \frac{\partial b}{\partial J} \quad (2.56)$$

in terms of the angle-action coordinates. The linearized Vlasov equation can be written also in terms of the angle-action coordinates as follows,

$$\frac{\partial f_1}{\partial t} + \Omega(J) \frac{\partial f_1}{\partial \theta} - f_0'(J) \frac{\partial}{\partial \theta} \mathcal{V}[f_1] = 0, \quad (2.57)$$

where $\Omega(J) = d\mathcal{H}[f_0](J)/dJ$. We expand the functions $f_1(\theta, J, t)$, $\cos q(\theta, J)$, and $\sin q(\theta, J)$ into the Fourier series,

$$f_1(\theta, J, t) = \sum_{k \in \mathbb{Z}} f_{1,k}(J, t) e^{ik\theta}, \quad (2.58)$$

$$\cos q(\theta, J) = \sum_{k \in \mathbb{Z}} C^k(J) e^{ik\theta}, \quad (2.59)$$

$$\sin q(\theta, J) = \sum_{k \in \mathbb{Z}} S^k(J) e^{ik\theta}, \quad (2.60)$$

respectively. By using Eqs. (2.58), (2.59), and (2.60), the potential term $\mathcal{V}[f_1]$ in Eq. (2.57) is written in the form,

$$\begin{aligned} -\mathcal{V}[f_1](q(\theta, J)) &= \iint_{\mu} \cos(q(\theta, J) - q'(\theta', J')) f_1(\theta', J', t) d\theta' dJ' \\ &= 2\pi \sum_{m \in \mathbb{Z}} C^m(J) e^{im\theta} \sum_{k \in \mathbb{Z}} \int_L C^k(J')^* f_{1,k}(J', t) dJ' \\ &\quad + 2\pi \sum_{m \in \mathbb{Z}} S^m(J) e^{im\theta} \sum_{k \in \mathbb{Z}} \int_L S^k(J')^* f_{1,k}(J', t) dJ'. \end{aligned} \quad (2.61)$$

Then, the m -th Fourier mode $f_{1,m}$ is shown to satisfy the equation,

$$\begin{aligned} \frac{\partial f_{1,m}}{\partial t} &= -im\Omega(J) f_{1,m}(J, t) \\ &\quad - 2\pi im C^m(J) f'_0(J) \sum_{k \in \mathbb{Z}} \int_L C^k(J')^* f_{1,k}(J', t) dJ' \\ &\quad - 2\pi im S^m(J) f'_0(J) \sum_{k \in \mathbb{Z}} \int_L S^k(J')^* f_{1,k}(J', t) dJ'. \end{aligned} \quad (2.62)$$

Let $f_1^\lambda(\theta, J, t) = \sum_{m \in \mathbb{Z}} f_{1,m}^\lambda(J, t) e^{im\theta}$ be an eigenfunction associated with the eigenvalue λ of $\widehat{\mathcal{L}}$, i.e., $(f_{1,m}^\lambda)_{m \in \mathbb{Z}}$ be the eigenvector associated with the eigenvalue λ . Setting

$$f_{1,m}^\lambda(J, t) = \tilde{f}_{1,m}^\lambda(J) e^{\lambda t}, \quad \forall m \in \mathbb{Z}, \quad (2.63)$$

and substituting it into Eq. (2.62), we get

$$\begin{aligned} \tilde{f}_{1,m}^\lambda(J) &= -2\pi \frac{mf'_0(J)}{m\Omega(J) - i\lambda} C^m(J) \sum_{k \in \mathbb{Z}} \int_L C^k(J')^* \tilde{f}_{1,k}^\lambda(J') dJ' \\ &\quad - 2\pi \frac{mf'_0(J)}{m\Omega(J) - i\lambda} S^m(J) \sum_{k \in \mathbb{Z}} \int_L S^k(J')^* \tilde{f}_{1,k}^\lambda(J') dJ'. \end{aligned} \quad (2.64)$$

Multiplying $C^m(J)^*$ or $S^m(J)^*$ to both sides of Eq. (2.64), summing up with respect to $m \in \mathbb{Z}$, and using the fact [BOY2010]

$$2\pi \sum_{m \in \mathbb{Z}} \int_L \frac{mf'_0(J)}{m\Omega(J) - i\lambda} C^m(J)^* S^m(J) dJ = 0, \quad (2.65)$$

we obtain the equations

$$\begin{aligned} \left[1 + 2\pi \sum_{m \in \mathbb{Z}} \int_L \frac{mf'_0(J)}{m\Omega(J) - i\lambda} |C^m(J)|^2 dJ \right] \sum_{k \in \mathbb{Z}} \int_L C^k(J')^* \tilde{f}_{1,k}^\lambda(J') dJ' &= 0, \\ \left[1 + 2\pi \sum_{m \in \mathbb{Z}} \int_L \frac{mf'_0(J)}{m\Omega(J) - i\lambda} |S^m(J)|^2 dJ \right] \sum_{k \in \mathbb{Z}} \int_L S^k(J')^* \tilde{f}_{1,k}^\lambda(J') dJ' &= 0. \end{aligned} \quad (2.66)$$

A necessary condition for the existence of the non-zero eigenfunction corresponding to the eigenvalue λ is that at least one of the following two equations is satisfied;

$$\begin{aligned}\Lambda_x(i\lambda) &\equiv 1 + 2\pi \sum_{m \in \mathbb{Z}} \int_L \frac{m f'_0(J)}{m\Omega(J) - i\lambda} |C^m(J)|^2 dJ = 0, \\ \Lambda_y(i\lambda) &\equiv 1 + 2\pi \sum_{m \in \mathbb{Z}} \int_L \frac{m f'_0(J)}{m\Omega(J) - i\lambda} |S^m(J)|^2 dJ = 0.\end{aligned}\tag{2.67}$$

We note that the domain of $\Lambda_x(\omega)$ and $\Lambda_y(\omega)$ is $\mathbb{C} \setminus \mathbb{R}$.

Dispersion relation We next consider the initial value problem (2.25) with an initial condition $f_1(J, \theta, 0) = g(J, \theta)$, i.e., $f_{1,k}(J, 0) = g_k(J)$ for $k \in \mathbb{Z}$. Taking the Laplace transformation of the both sides of Eq. (2.62), we get

$$\begin{aligned}\tilde{f}_{1,m}(J, \omega) + 2\pi m C^m(J) \frac{f'_0(J)}{m\Omega(J) - \omega} \sum_{k \in \mathbb{Z}} \int_L C^k(J')^* \tilde{f}_{1,m}(J, \omega) dJ' \\ + 2\pi m S^m(J) \frac{f'_0(J)}{m\Omega(J) - \omega} \sum_{k \in \mathbb{Z}} \int_L S^k(J')^* \tilde{f}_{1,m}(J, \omega) dJ' = \frac{g_m(J)}{i(m\Omega(J) - \omega)}.\end{aligned}\tag{2.68}$$

Multiplying $C^m(J)^*$ or $S^m(J)^*$ to the both sides of Eq. (2.68), summing up over $m \in \mathbb{Z}$, and using the fact (2.65) we can conclude that the nontrivial mode $\sim e^{i\omega t}$ arises when the dispersion relation

$$D_x(\omega) = 0, \text{ or } D_y(\omega) = 0\tag{2.69}$$

is satisfied where

$$\begin{aligned}D_x(\omega) &\equiv 1 + 2\pi \sum_{m \in \mathbb{Z}} \int_L \frac{m f'_0(J)}{m\Omega(J) - \omega} |C^m(J)|^2 dJ, \\ D_y(\omega) &\equiv 1 + 2\pi \sum_{m \in \mathbb{Z}} \int_L \frac{m f'_0(J)}{m\Omega(J) - \omega} |S^m(J)|^2 dJ.\end{aligned}\tag{2.70}$$

The domain of the dispersion function is the upper half ω plane, but can be extended to the whole ω plane as for the homogeneous case (2.37). We note that the dispersion functions $D_x(\omega)$ and $D_y(\omega)$ have log-singularities which come from the fact that the integral interval with respect to dJ in Eq. (2.70) has an end point at $J = 0$. So does the function $G_m(\omega)$ given by

$$G_m(\omega) = \int_L \frac{g_m(J)}{i(m\Omega(J) - \omega)} dJ.\tag{2.71}$$

These log-singularities induce algebraic dampings to the inhomogeneous stationary state [BOY2011].

Let us compare the dispersion functions $D_x(\omega)$ and $D_y(\omega)$ with the spectral functions $\Lambda_x(\omega)$ and $\Lambda_y(\omega)$ respectively. When $\text{Im}\omega > 0$, the spectral functions $\Lambda_x(\omega)$ and $\Lambda_y(\omega)$ defined in Eq. (2.67) respectively coincide with the dispersion functions $D_x(\omega)$ and $D_y(\omega)$ which are defined in Eq. (2.70). As in the homogeneous case, both $\Lambda_x(\omega)$ and $\Lambda_y(\omega)$ satisfy the relation (2.32), since $|C^m(J)| = |C^{-m}(J)|$ and $|S^m(J)| = |S^{-m}(J)|$ are satisfied for all $m \in \mathbb{Z}$. The dispersion functions $D_x(\omega)$ and $D_y(\omega)$ satisfy the relation $D_i(-\omega^*) = D_i(\omega)^*$ ($i = x, y$).

2.5 Generalized Hamiltonian mean-field model

Let us consider the dynamical systems on a one-dimensional lattice with Hamiltonian,

$$H_N = \sum_{i=1}^N \frac{p_i^2}{2} + \frac{1}{2} \sum_{i,j=1}^N K_N(r_i - r_j) (1 - \cos(q_i - q_j)) - \sum_{i=1}^N h(r_i) \cos q_i, \quad (2.72)$$

where r_i is the i -th lattice point, the lattice spacing is set as $r_{i+1} - r_i = 1/N$, $q_i \in [-\pi, \pi)$ and $p_i \in \mathbb{R}$, for all $i = 1, 2, \dots, N$. We put $r_N = 1/2$ and we assume the periodic boundary condition for the lattice by identifying r_0 with r_N . The interaction term $K_N(r)$ is assumed to satisfy

$$K_N(0) = 0, \quad K_N(r) \geq 0, \quad K_N(r) = K_N(-r) \quad (2.73)$$

for all $r \in (-1/2, 1/2]$. The interaction $K_N(r)$ is also assumed to be normalized as

$$\sum_{i=1}^N K_N(r_i) = 1, \quad (2.74)$$

so that system has the extensivity [KUH1963]. In the equilibrium states, the mean-field theory is exact in the thermodynamic limit $N \rightarrow \infty$ for such a generalized HMF model [Mor2010].

Example. If we put the site-site interaction $K_N(r)$ as

$$K_{N,\alpha}(r_i - r_j) = \frac{\kappa_{N,\alpha}}{\|r_i - r_j\|^\alpha}, \quad 0 \leq \alpha < 1, \quad \|r\| \equiv \min\{|r|, 1 - |r|\}, \quad (2.75)$$

the model (2.72) becomes the α -HMF model [AT1998]. The parameter $\kappa_{N,\alpha}$ is set so that $K_{N,\alpha}$ satisfies the condition (2.74).

Taking a limit $N \rightarrow \infty$, we get the effective single-body Hamiltonian

$$\begin{aligned} \mathcal{H}_r[f] &= \frac{p^2}{2} + \mathcal{V}_r[f](q, t), \\ \mathcal{V}_r[f](q, t) &= - \int_{-1/2}^{1/2} dr' K(r - r') \iint_{\mu} \cos(q - q') f(q', p', r', t) dq dp - h(r) \cos q, \end{aligned} \quad (2.76)$$

by using the procedure exhibited in Ref. [BDN+2011], where f denotes the single-body distribution, and μ denotes the whole μ space, $S^1 \times \mathbb{R}$. The interaction term $K(r)$ in Eq. (2.76) in the limit of $N \rightarrow \infty$ is given by

$$K(r) = \lim_{N \rightarrow \infty} K_N(r), \quad (2.77)$$

so that it satisfies

$$\int_{-1/2}^{1/2} K(r) dr = 1. \quad (2.78)$$

The single-body distribution $f(q, p, r, t)$ is a solution to the Vlasov equation

$$\frac{\partial f}{\partial t} + \{\mathcal{H}_r[f], f\} = 0, \quad (2.79)$$

for each configuration r on the lattice. Thanks to the periodicity of the lattice, $K(r)$ can be expanded into the Fourier series as

$$K(r) = \sum_{n \in \mathbb{Z}} K_n e^{2\pi i n r}. \quad (2.80)$$

When the stationary state f_0 in question and the external field $h(r)$ are independent from r , so is the effective single-body Hamiltonian $\mathcal{H}_r[f_0]$ and so are the associated angle-action variables (θ, J) . The linearized Vlasov equation is derived from Eq. (2.79) as

$$\begin{aligned} \frac{\partial f_1}{\partial t} &= \widehat{\mathcal{L}}_r[f_1], \\ \widehat{\mathcal{L}}_r[f_1] &= -\{\mathcal{H}_r[f_0], f_1\} - \{\mathcal{V}[f_1], f_0\}. \end{aligned} \quad (2.81)$$

This equation can be analyzed by means of the Fourier transformation with respect to r , the Fourier transformation with respect to q or θ , and the Laplace transformation with respect to t . Using the same procedure exhibited in the last section, we can derive the dispersion functions as

$$\begin{aligned} D_x^n(\omega) &= 1 + 2\pi K_n \sum_{m \in \mathbb{Z}} \int_L \frac{m f_0'(J)}{m \Omega(J) - \omega} |C^m(J)|^2 dJ, \\ D_y^n(\omega) &= 1 + 2\pi K_n \sum_{m \in \mathbb{Z}} \int_L \frac{m f_0'(J)}{m \Omega(J) - \omega} |S^m(J)|^2 dJ, \end{aligned} \quad (2.82)$$

for $n \in \mathbb{Z}$.

Chapter 3

Stability criteria of stationary solutions to the Vlasov equation for the Hamiltonian mean-field model

3.1 Introduction

Finding a stability criterion for stationary solutions to the Vlasov equation is the first step to investigate QSSs, since such a criterion makes it possible to decide whether a stationary solution can be a QSS or not. This is because the QSSs are supposed to be associated with stable stationary solutions to the Vlasov equation [BT2008, YBB+2004, BBD+2006, CDR2009].

The stability of solutions to the Vlasov equation has been investigated in Refs. [BT2008, Pen1960, Ant1960, HMRW1985, Kan1990, Kan1991, IK1993, YBB+2004, BBD+2006, CD2009, CC2010, LMR2012]. There are several concepts of stability such as the spectral stability, the linear stability, the formal stability, and the nonlinear stability [HMRW1985]. The interest of this paper centers on the spectral stability and the formal stability, but the linear stability and the nonlinear stability are not touched upon. The formal [HMRW1985, YBB+2004] and spectral [Pen1960, CD2009, IK1993] stability criteria for spatially homogeneous solutions have been well known already.

Meanwhile, the stability of spatially inhomogeneous solutions has been investigated in the astrophysics [Ant1960, BT2008, Kan1990, Kan1991] since around a half century ago. The stability for the spherical galaxy is rigorously investigated recently [LMR2012]. Antonov's variational principle [BT2008, Ant1960] particularly gives a necessary and sufficient condition for stability of some stationary solution by considering stability against not all perturbations but only accessible perturbations called phase preserving perturbations [Kan1991]. The restriction for the perturbations comes from the fact that the Vlasov equation has an infinite number of invariants. We note that the stability of a given stationary state cannot be determined by using the stability criterion given in a statement of Antonov's variational principle [BT2008] practically.

In the context of statistical physics for QSSs, the stability of spatially inhomogeneous solutions to the Vlasov equation has been studied, say, by Campa and Chavanis [CC2010]. They set up criteria for formal stability both in the most refined form and in less refined forms, by using the fact that accessible perturbations conserve all Casimir invariants (2.22) at linear order. We call the most refined formal stability, simply, the formal stability in this paper. Their formal

stability criterion in the most refined form requires one to take into account an infinite number of Casimir invariants and to detect an infinite number of associated Lagrange multipliers in order to determine the stability of spatially inhomogeneous stationary solutions. Their formal stability criterion is hence hard to use. In contrast with this, the canonical formal stability criterion which is one of the less refined formal stability criteria is of practical use. Using the canonical formal stability criterion, one can check stability of a stationary state against a perturbation which keeps the normalization condition but may break the energy conservation and other Casimir invariant conditions. Although the criterion for canonical formal stability is stated as a necessary and sufficient condition, it is just a sufficient condition for the formal stability. It is to be expected that a criterion for the formal stability is found out in the form of necessary and sufficient condition without reference to an infinite number of quantities such as Lagrange multipliers.

This chapter deals with the Hamiltonian mean-field (HMF) model [MS1982, AR1995] with the anticipation stated above. The HMF model is a simple toy model which shows typical long-range features as we mentioned in Chapter 2. Moreover, the HMF model allows one to perform theoretical study on dynamics near spatially inhomogeneous stationary solutions to the Vlasov equation by the use of the dispersion function which can be explicitly written out for the HMF model. For instance, the dynamics of a perturbation around the spatially inhomogeneous stationary solution [BOY2010] and the algebraic damping to a QSS [BOY2011] have been investigated theoretically and numerically by using the HMF model. Further, the linear response to the external field is studied in an explicit form [OY2012] for a spatially inhomogeneous QSS. In those studies, the stability of the spatially inhomogeneous solutions have been assumed to hold, and then it is worthwhile to give an explicit form of necessary and sufficient condition for the stability of the spatially inhomogeneous stationary solutions. The aim of this chapter is to find spectral and formal stability criteria for spatially inhomogeneous stationary solutions. The spectral stability criterion is derived by means of the dispersion relation. The formal stability criterion is obtained by using the same idea as exhibited in Ref. [CC2010]. The criterion we are to find by using the angle-action variables is free from an infinite number of Lagrange multipliers, and is stated in the form of a necessary and sufficient condition, which allows us to look into the stability of spatially inhomogeneous solutions in an accessible manner.

This chapter is organized as follows. Section 3.2 contains a brief review of the two kinds of stabilities of a fixed point of a dynamical system. The spectral stability criterion for spatially homogeneous solutions to the Vlasov equation is given in Section 3.3 in a rather simple method than that already known. By using the same method, the spectral stability criterion for spatially inhomogeneous solutions is obtained in Section 3.4.1. The formal stability criterion for spatially inhomogeneous solutions is derived in Section 3.4.3. In Section 3.4.4, we look into stability of a spatially inhomogeneous waterbag distribution by using the obtained criterion. Section 3.5 gives an example which shows that the present stability criterion is of great use. It is shown that there is a family of stationary solutions whose stability cannot be judged correctly by using the canonical formal stability criterion but can be done by the criterion given in this chapter. Section 3.6 is devoted to a summary and a discussion for generalization.

3.2 Spectral stability and formal stability

We start with a brief review of definitions of spectral stability and formal stability, following Holm et al. [HMRW1985]. Let X be a normed space. Suppose that a dynamical system is given by the equation,

$$\frac{dx}{dt} = f(x), \quad x \in X. \quad (3.1)$$

Let x_* be a fixed point of this system, $f(x_*) = 0$. Then, the linearized equation around x_* is expressed as

$$\frac{d\xi}{dt} = Df(x_*)[\xi], \quad (3.2)$$

where $Df(x_*)$ is a linear operator derived from f at x_* . The spectral stability and the formal stability of the fixed point x_* are defined as follows:

- The fixed point x_* is said to be *spectrally stable*, if the linear operator $Df(x_*)$ has no spectrum with positive real part. In addition, if the linear operator $Df(x_*)$ has an eigenvalue with vanishing real part, x_* is called *neutrally spectrally stable*. The fixed point x_* is said to be spectrally unstable when there exists a spectrum with positive real part.
- The fixed point x_* is said to be *formally stable*, if a conserved functional $\mathcal{F}[x]$ takes a critical value at $x = x_*$ and further the second variation of \mathcal{F} at x_* is negative (or positive) definite. The fixed point x_* is said to be neutrally formally stable if the second variation of \mathcal{F} at x_* is negative (resp. positive) semi-definite but not negative (resp. positive) definite. Further, the fixed point x_* said to be formally unstable if the second variation of \mathcal{F} at x_* is not negative (or positive) semi-definite.

We note that the formal stability can be defined for x^* which is a critical point of \mathcal{F} under some constraints coming from invariants of the dynamical system in question.

If the dynamical system in question is infinite-dimensional, the fixed point x_* is occasionally called a stationary state. We note that the definition of neutral spectral stability is different from the original one in Ref. [HMRW1985]. The detail of our footing for stability analysis is as follows: The neutral spectral stability is defined in terms of eigenvalues with vanishing real parts in Section 3.2. However, the neutral spectral stability is originally defined in terms of spectra, not eigenvalues only, with vanishing real parts [HMRW1985]. The reason why we modify the definition of neutral stability is that the linear operator $\widehat{\mathcal{L}}$ in Eq. (2.23) has always continuous spectrum on the imaginary axis, and this does not bring about spectral instability.

According to Ref. [HMRW1985], the neutrally spectrally stable solution is spectrally stable, but the neutrally formally stable solution is not formally stable.

We note that the linear stability and the spectral stability are different concepts. Then, it is worthwhile to exhibit a definition of the linear stability here:

- The fixed point x_* is said to be *linearly stable*, if and only if a solution $\xi(t)$ to the linearized equation (3.2) with initial condition $\xi(0)$ satisfies a condition,

$$\forall \epsilon > 0, \exists \delta > 0, \text{ such that } \|\xi(0)\| < \delta \Rightarrow \|\xi(t)\| < \epsilon, \quad (3.3)$$

where $\|\bullet\|$ is a norm.

3.3 Stability criteria for spatially homogeneous stationary solutions

As long as the linear operator $\widehat{\mathcal{L}}$ defined in Eq. (2.23) is concerned, the spectral stability condition for a stationary solution f_0 to the Vlasov equation can be compactly stated; if there is no eigenvalue of $\widehat{\mathcal{L}}$, the stationary solution f_0 is said to be spectrally stable. Since the spectrum of $\widehat{\mathcal{L}}$ consist of eigenvalues on $\mathbb{C} \setminus i\mathbb{R}$, continuous spectra on the imaginary axis, and the embedded eigenvalue on the imaginary axis [CH1989], only the eigenvalues are able to contribute to the spectral instability. On account of this fact, the spectral stability criterion is stated as follows:

Proposition 1 *Let $f_0(p)$ be a spatially homogeneous stationary solution to the Vlasov equation, which is assumed to be smooth, even, and unimodal, and further the derivative $f'_0(p)$ of which is assumed to have the support \mathbb{R} . Then, the stationary solution f_0 is spectrally stable, if and only if f_0 satisfies the inequality*

$$\mathcal{I}[f_0] = 1 + \pi \int_{-\infty}^{\infty} \frac{f'_0(p)}{p} dp \geq 0. \quad (3.4)$$

We note that $f'_0(p)/p$ has no singularity for all $p \in \mathbb{R}$ on account of the assumption that f_0 is smooth and even. Though the inequality (3.4) can be derived by using the Nyquist's method [CD2009, IK1993, Pen1960], we introduce a method other than the Nyquist's method to prove this proposition.

For a spatially homogeneous stationary solution $f_0(p)$, the dispersion relation $D(\omega) = 0$ with $\text{Im}\omega > 0$ is put in the form [CDR2009]

$$D(\omega) = 1 + \pi \int_{-\infty}^{\infty} \frac{f'_0(p)}{p - \omega} dp = 0, \quad \text{Im}\omega > 0. \quad (3.5)$$

The dispersion function is continued to $\omega = 0$ from the upper half ω plane, by taking the limit $D(0) = \lim_{\epsilon \rightarrow 0+} D(i\epsilon)$. Noting that $f'_0(p)/p$ has no singularity, we obtain $D(0) = \mathcal{I}[f_0]$, since the integrand in Eq. (3.5) has no singularity when $\omega = 0$. We put $\omega \in \mathbb{C}$ in the form $\omega = \omega_r + i\omega_i$ with $\omega_r \in \mathbb{R}$ and $\omega_i > 0$. When the dispersion relation (3.5) is satisfied by some ω with $\text{Im}\omega > 0$, the imaginary part of $D(\omega)$ is zero, so that one has

$$\begin{aligned} \text{Im}D(\omega) &= \pi\omega_i \int_{-\infty}^{\infty} \frac{f'_0(p)}{(p - \omega_r)^2 + \omega_i^2} dp \\ &= 4\pi\omega_i\omega_r \int_0^{\infty} \frac{pf'_0(p) dp}{((p - \omega_r)^2 + \omega_i^2)((p + \omega_r)^2 + \omega_i^2)} \\ &= 0. \end{aligned} \quad (3.6)$$

Since $f_0(p)$ is an even unimodal function, $pf'_0(p) < 0$ for all $p > 0$. The integral in Eq. (3.6) is to be negative value, and Eq. (3.6) implies that $\omega_r = 0$, since $\omega_i > 0$. Conversely, if $\omega_r = 0$, the equality $\text{Im}D(\omega) = 0$ holds true. The condition $\omega_r = 0$ is then equivalent to the condition (3.6).

Now, on account of the fact $pf'_0(p)$ is negative for all $p \neq 0$, and the dispersion function satisfies the inequality

$$D(i\omega_i) = 1 + \pi \int_{-\infty}^{\infty} \frac{pf'_0(p)}{p^2 + \omega_i^2} dp \geq \mathcal{I}[f_0], \quad (3.7)$$

for all $\omega_i \geq 0$, where the equality is satisfied if and only if $\omega_i = 0$. This is because $D(i\omega_i)$ becomes $\mathcal{I}[f_0]$ for $\omega_i = 0$ and because $D(i\omega_i)$ is a continuous and strictly increasing function with respect to ω_i . It then follows that if $D(\omega) = 0$ with $\omega = i\omega_i$, or equivalently, if $\widehat{\mathcal{L}}$ has an eigenvalue $-i\omega$ with $\text{Im}\omega > 0$, then $\mathcal{I}[f_0] < 0$. Conversely, if the inequality $\mathcal{I}[f_0] < 0$ is satisfied, there exists a positive ω_i such that $D(i\omega_i) = 0$. In fact, $D(i\omega_i)$ is strictly increasing in ω_i with $D(0) = \mathcal{I}[f_0]$ and $D(i\omega_i) \rightarrow 1$ as $\omega_i \rightarrow \infty$. This means that $\widehat{\mathcal{L}}$ has an unstable eigenvalue if and only if $\mathcal{I}[f_0] < 0$. Thus we have proved the spectral stability criterion (3.4).

In comparison with the spectral stability criterion (3.4), the formal stability criterion [YBB+2004] is given by

$$\mathcal{I}[f_0] > 0. \quad (3.8)$$

This inequality means that f_0 is spectrally stable but not neutrally spectrally stable. This is because if $D(0) = \mathcal{I}[f_0] = 0$, the linear operator $\widehat{\mathcal{L}}$ has an embedded eigenvalue 0, and hence f_0 is neutrally spectrally stable.

3.4 Stability criteria for spatially inhomogeneous stationary solutions

In this section, we will give necessary and sufficient conditions for the spectral stability and for the most refined formal stability of spatially inhomogeneous stationary solutions to the Vlasov equation. We call the most refined formal stability, simply, the formal stability as we have already mentioned in the introduction.

A spectral stability criterion for spatially inhomogeneous solutions can be given in an explicit form by performing the same procedure as that adopted in the last section.

Furthermore, the formal stability criterion can be worked out if all the Casimir invariants (2.22) are taken into account. For spatially inhomogeneous stationary solutions, Campa and Chavanis [CC2010] have given the formal stability criterion. However, no one has these criteria explicitly, since one needs to detect values of an infinite number of Lagrange multipliers. We can avoid a puzzle to detect an infinite number of Lagrange multipliers if we use the angle-action coordinates in stability analysis.

We denote the single-body energy by

$$\mathcal{E}(q, p) = \frac{p^2}{2} - M_0 \cos q, \quad (3.9)$$

where on account of the rotational symmetry of the HMF model, the order parameter has been set $\vec{M}_0 = (M_0, 0)$ with

$$M_0 = \iint_{\mu} \cos q f_0(q, p) dq dp. \quad (3.10)$$

3.4.1 Spectral stability criterion

We derive a necessary and sufficient condition for a spatially inhomogeneous stationary solution f_0 to the Vlasov equation to be spectrally stable, which is stated as follows:

Proposition 2 *Let f_0 be a spatially inhomogeneous stationary solution to the Vlasov equation, which is assumed to depend on the action J only through the single-body energy $\mathcal{E}(J)$ in such a manner that*

$$f_0(q, p) = \tilde{f}_0(J(q, p)) = \hat{f}_0(\mathcal{E}(q, p)). \quad (3.11)$$

Further, $\tilde{f}_0(J)$ and $\hat{f}_0(\mathcal{E})$ are assumed to be strictly decreasing with respect to J and \mathcal{E} , respectively. A further assumption is that $d\hat{f}_0(\mathcal{E})/d\mathcal{E}$ is continuous with respect to \mathcal{E} . Such a stationary solution $f_0(q, p)$ is spectrally stable, if and only if

$$\mathcal{I}[f_0] = 1 + \int_{-\pi}^{\pi} dq \cos^2 q \int_{-\infty}^{\infty} \frac{1}{p} \frac{\partial f_0}{\partial p}(q, p) dp - 2\pi \int_L \frac{\tilde{f}'_0(J)}{\Omega(J)} |C^0(J)|^2 dJ \geq 0, \quad (3.12)$$

where (θ, J) are the angle-action coordinates and $\Omega(J) \equiv d\mathcal{E}(J)/dJ$, and where $C^n(J)$ is defined by

$$C^n(J) \equiv \frac{1}{2\pi} \int_{-\pi}^{\pi} \cos q(\theta, J) e^{-in\theta} d\theta, \quad n \in \mathbb{Z}. \quad (3.13)$$

Before proving Prop. 2, we note that all distributions such as (3.11) are stationary solutions to the Vlasov equation. The monotonicity of f_0 in J is satisfied for stationary solutions which are obtained as solutions to a variational equation associated with an optimization problem such as the maximization of the entropy or the minimization of the free energy. Then, the assumption imposed on f_0 in Prop. 2 is not too restrictive, and has some physical relevance. We note also that $\tilde{f}'_0(J)/\Omega(J)$ is finite for all J since $d\hat{f}_0(\mathcal{E})/d\mathcal{E}$ has no singularity.

The proof of Prop. 2 can be performed in a similar manner to that applied to Prop. 1, though the f_0 is spatially inhomogeneous in the present proof. We divide the stability analysis into two, one of which deals with stability against the perturbation in the direction parallel to the order parameter $\vec{M}_0 = (M_0, 0)^T$ and the other with stability against the perturbation in the direction perpendicular to \vec{M}_0 .

We first analyze the stability against the perturbation in the direction parallel to the order parameter $\vec{M}_0 = (M_0, 0)^T$. The dispersion function in this case is put in the form (2.70)

$$D_x(\omega) = 1 + 2\pi \sum_{m \in \mathbb{Z}} \int_L \frac{m \tilde{f}'_0(J)}{m \Omega(J) - \omega} |C^m(J)|^2 dJ, \quad \text{Im} \omega > 0, \quad (3.14)$$

and the dispersion relation is given by $D_x(\omega) = 0$ [BOY2010]. As we have reviewed in Section 2.4.2, the stationary solution f_0 is spectrally unstable if and only if the dispersion relation has a root in the upper half ω plane. When $\text{Im} \omega > 0$, the term of $m = 0$ in Eq. (3.14) vanishes and Eq. (3.14) is arranged as

$$D_x(\omega) = 1 + 2\pi \sum_{m \in \mathbb{Z} \setminus \{0\}} \int_L \frac{\tilde{f}'_0(J)}{\Omega(J) - \omega/m} |C^m(J)|^2 dJ, \quad \text{Im} \omega > 0. \quad (3.15)$$

We here note that $D_x(0)$ is defined as $D_x(0) = \lim_{\epsilon \rightarrow 0+} D_x(i\epsilon)$, and

$$D_x(0) = 1 + 2\pi \sum_{m \neq 0} \int_L \frac{\tilde{f}'_0(J)}{\Omega(J)} |C^m(J)|^2 dJ, \quad (3.16)$$

since the integrand in it has no singularity.

If there exists ω such that $D_x(\omega) = 0$ with $\text{Im}\omega > 0$, then one has $\text{Im}D_x(\omega) = 0$, which is written out as

$$\begin{aligned} \text{Im}D_x(\omega) &= \sum_{m \in \mathbb{Z} \setminus \{0\}} \frac{2\pi}{m} \omega_i \int_L \frac{|C^m(J)|^2 \Omega(J) \tilde{f}'_0(J)}{(\Omega(J) - \omega_r/m)^2 + (\omega_i/m)^2} dJ \\ &= \sum_{m \in \mathbb{N}} \left[\frac{2\pi}{m} \omega_i \int_L \frac{|C^m(J)|^2 \Omega(J) \tilde{f}'_0(J)}{(\Omega(J) - \omega_r/m)^2 + (\omega_i/m)^2} dJ - \frac{2\pi}{m} \omega_i \int_L \frac{|C^{-m}(J)|^2 \Omega(J) \tilde{f}'_0(J)}{(\Omega(J) + \omega_r/m)^2 + (\omega_i/m)^2} dJ \right] \\ &= \sum_{m \in \mathbb{N}} \frac{8\pi}{m} \omega_r \omega_i \int_L \frac{|C^m(J)|^2 \Omega(J) \tilde{f}'_0(J)}{\{(\Omega(J) - \omega_r/m)^2 + (\omega_i/m)^2\} \{(\Omega(J) + \omega_r/m)^2 + (\omega_i/m)^2\}} dJ = 0, \end{aligned} \quad (3.17)$$

where we have used the fact $C^m(J) = C^{-m}(J)^*$ which is derived from Eq. (3.13). Since $|C^m(J)|^2 > 0$ for some $m \in \mathbb{N}$, and $\Omega(J) > 0$ and $\tilde{f}'_0(J) < 0$ for all J , the integrals in Eq. (3.17) give negative values. Then, Eq. (3.17) yields $\omega_r = 0$, since $\omega_i > 0$. We thus have shown that if $\omega = \omega_r + i\omega_i$ with $\omega_i > 0$ is a root of $D_x(\omega) = 0$ then $\omega_r = 0$.

On account of $\omega_r = 0$, the dispersion relation reduces to

$$\begin{aligned} D_x(i\omega_i) &= 1 + 4\pi \sum_{m \in \mathbb{N}} \int_L \frac{\Omega(J) \tilde{f}'_0(J)}{\Omega(J)^2 + (\omega_i/m)^2} |C^m(J)|^2 dJ \\ &= 0. \end{aligned} \quad (3.18)$$

The function $D_x(i\omega_i)$ is a strictly increasing continuous function of ω_i , and converges to 1, $D_x(i\omega_i) \rightarrow 1$, as $\omega_i \rightarrow \infty$. This implies that if $D_x(0) < 0$, there is a positive number $\omega_i > 0$ such that $D_x(i\omega_i) = 0$. Put another way, if $D_x(0) < 0$, there is an ω such that $D_x(\omega) = 0$, $\text{Im}\omega > 0$. The converse is also shown by taking the contraposition of that there is no root ω of $D(\omega)$ with $\text{Im}\omega > 0$ if $D_x(0) \geq 0$. We hence conclude that there is no unstable eigenvalue for the perturbation whose direction is parallel to the order parameter $\vec{M}_0 = (M_0, 0)^T$, if and only if $D_x(0) \geq 0$. If $D_x(0) = 0$, the operator $\hat{\mathcal{L}}$ has an embedded eigenvalue 0, so that f_0 is neutrally spectrally stable.

To derive the spectral stability criterion (3.12), we have only to prove the relation, $D_x(0) = \mathcal{I}[f_0]$. According to Eq. (2.49), the function $\cos q$ is expressed as (2.51). Owing to the periodicity of the Jacobian elliptic functions [WW1927], the function $\cos q(\theta, J)$ is 2π -periodic with respect to θ . Then, from Parseval's equality, we obtain

$$2\pi \sum_{m \neq 0} |C^m(J)|^2 = \int_{-\pi}^{\pi} \cos^2 q(\theta, J) d\theta - 2\pi |C^0(J)|^2. \quad (3.19)$$

By using this equation, we rewrite the second terms in the right-hand side of Eq. (3.16) as

$$\int_L dJ \frac{\tilde{f}'_0(J)}{\Omega(J)} \int_{-\pi}^{\pi} \cos^2 q(\theta, J) d\theta - 2\pi \int_L \frac{\tilde{f}'_0(J)}{\Omega(J)} |C^0(J)|^2 dJ. \quad (3.20)$$

Keeping in mind the fact that the stationary solution f_0 to the Vlasov equation depends on the action J only through a single-body energy \mathcal{E} , we arrange the first term of (3.20) as

$$\begin{aligned} \int_L dJ \frac{\tilde{f}'_0(J)}{\Omega(J)} \int_{-\pi}^{\pi} \cos^2 q(\theta, J) d\theta &= \int_L dJ \int_{-\pi}^{\pi} \frac{d\hat{f}_0}{d\mathcal{E}}(\mathcal{E}(J)) \cos^2 q(\theta, J) d\theta \\ &= \iint_{\mu} \frac{d\hat{f}_0}{d\mathcal{E}}(\mathcal{E}(J)) \cos^2 q(\theta, J) d\theta dJ \\ &= \iint_{\mu} \frac{1}{p} \frac{\partial f_0}{\partial p}(q, p) \cos^2 q dq dp. \end{aligned} \quad (3.21)$$

In the course of analysis, we have used the fact that the transformation $(\theta, J) \mapsto (q, p)$ is canonical. We note that $d\hat{f}_0/d\mathcal{E}$ is assumed to be continuous in J , and hence the integration with respect to J is taken along on the real J axis. Then, by using Eqs. (2.54) and (2.55), the second equality in Eq. (3.21) is derived. Equations (3.16), (3.20), and (3.21) are put together to show the relation $D_x(0) = \mathcal{I}[f_0]$.

So far we have investigated the stability against perturbations in the direction parallel to the order parameter $\vec{M}_0 = (M_0, 0)^T$. We proceed to look into the stability against a perturbation in the direction perpendicular to the order parameter \vec{M}_0 . The dispersion relation corresponding to the direction perpendicular to the order parameter \vec{M}_0 is expressed as

$$D_y(\omega) = 1 + 2\pi \sum_{m \in \mathbb{Z}} \int_L \frac{m \tilde{f}'_0(J)}{m\Omega(J) - \omega} |S^m(J)|^2 dJ = 0, \quad (3.22)$$

for $\text{Im}\omega > 0$, where

$$S^m(J) \equiv \frac{1}{2\pi} \int_{-\pi}^{\pi} \sin q(\theta, J) e^{-im\theta} d\theta. \quad (3.23)$$

We note that $S^0(J) = 0$. In fact, $\sin q(\theta, J)$ is expressed as (2.50), and it is odd with respect to θ for all J [WW1927], so that one has $S^0(J) = 0$.

Following the same procedure as that for proving the relation $D_x(0) = \mathcal{I}[f_0]$ and taking into account the relation $S^0(J) = 0$, we obtain

$$D_y(0) = 1 + \iint_{\mu} \frac{1}{p} \frac{\partial f_0}{\partial p}(q, p) \sin^2 q dq dp. \quad (3.24)$$

If $D_y(0) \geq 0$, there is no eigenmode which brings about the instability in a direction perpendicular to the order parameter \vec{M}_0 . Actually, the equality, $D_y(0) = 0$, is satisfied for any stationary solution subject to the assumptions in Prop. 2 with (3.9), which is proved as follows [CC2010];

$$\begin{aligned} \iint_{\mu} \frac{1}{p} \frac{\partial f_0}{\partial p}(q, p) \sin^2 q dq dp &= \iint_{\mu} \frac{d\hat{f}_0}{d\mathcal{E}}(\mathcal{E}(q, p)) \sin^2 q dq dp \\ &= \frac{1}{M_0} \iint_{\mu} \frac{\partial f_0}{\partial q}(q, p) \sin q dq dp \\ &= -\frac{1}{M_0} \iint_{\mu} f_0(q, p) \cos q dq dp = -1. \end{aligned} \quad (3.25)$$

Since $D_x(0) = \mathcal{I}[f_0]$ and $D_y(0) = 0$, we have obtained the spectral stability criterion (3.12) for the spatially inhomogeneous solutions to the Vlasov equation. It is to be remarked that any spectrally stable solution which are spatially inhomogeneous are neutrally spectrally stable, since there is an embedded eigenvalue 0 which comes from $D_y(0) = 0$.

To compute $D_x(0)$ or the right-hand side of (3.12), we should express the term including $C^0(J)$ in terms of known functions. Using the explicit expression (2.52) of $\Omega(J)$ and the expressions (B.2) and (B.3) in Appendix B of $C_0(J)$, we obtain

$$\begin{aligned} 2\pi \int_L \frac{f'_0(J)}{\Omega(J)} |C^0(J)|^2 dJ &= \frac{1}{2\pi} \int_0^\infty dk \frac{1}{\Omega(k)} \frac{d\bar{f}_0}{dk}(k) \left(\int_{-\pi}^\pi \cos^2 q(\theta, J(k)) d\theta \right)^2 \\ &= \frac{4}{\sqrt{M_0}} \int_1^\infty \frac{K(1/k)}{k} \left(\frac{2k^2 E(1/k)}{K(1/k)} + 1 - 2k^2 \right)^2 \frac{d\bar{f}_0}{dk}(k) dk \\ &\quad + \frac{4}{\sqrt{M_0}} \int_0^1 K(k) \left(\frac{2E(k)}{K(k)} - 1 \right)^2 \frac{d\bar{f}_0}{dk}(k) dk. \end{aligned} \quad (3.26)$$

Then, $D_x(0)$ is described explicitly as

$$\begin{aligned} D_x(0) &= 1 + \iint_\mu \frac{1}{p} \frac{\partial f_0}{\partial p}(q, p) \cos^2 q dq dp \\ &\quad - \frac{4}{\sqrt{M_0}} \int_0^1 K(k) \left[\frac{2E(k)}{K(k)} - 1 \right]^2 \bar{f}'_0(k) dk \\ &\quad - \frac{4}{\sqrt{M_0}} \int_1^\infty \frac{K(1/k)}{k} \left[\frac{2k^2 E(1/k)}{K(1/k)} + 1 - 2k^2 \right]^2 \bar{f}'_0(k) dk, \end{aligned} \quad (3.27)$$

where $\bar{f}_0(k) \equiv \bar{f}_0(J(k))$, and where $E(k)$ is the complete elliptic integral of the second kind [WW1927].

3.4.2 Stationary states realized as critical points of some invariant functionals

We will give a necessary and sufficient condition of the formal stability of a stationary state. To look into the formal stability, we introduce invariant functionals.

As we remarked in Section 2.3, the Vlasov dynamics satisfies the normalization condition

$$\mathcal{N}[f] \equiv \iint_\mu f(q, p) dq dp = 1, \quad (3.28)$$

the momentum conservation law

$$\mathcal{P}[f] \equiv \iint_\mu p f(q, p) dq dp = 0, \quad (3.29)$$

and the energy conservation law

$$\mathcal{U}[f] \equiv \iint_\mu \frac{p^2}{2} f(q, p) dq dp - \frac{1}{2} (M_x[f]^2 + M_y[f]^2) = U, \quad (3.30)$$

where U is a fixed value. The Vlasov dynamics additionally has an infinite number of Casimir invariants denoted by

$$\mathcal{S}[f] = \iint_{\mu} s(f(q, p)) dq dp. \quad (3.31)$$

We here assume that s is a strictly concave and twice differentiable function defined for the non-negative real numbers.

We will look into the formal stability of the stationary solution realized as the critical point of the functional (3.31) under constraints (3.28), (3.29), and (3.30). A critical point $\tilde{f}_0(J)$ is a solution to the variational equation

$$\delta\mathcal{F} = \delta(\mathcal{S} - \beta\mathcal{U} - \alpha\mathcal{N}) = 0, \quad (3.32)$$

which is written out as

$$s'(\tilde{f}_0(J)) = \beta\mathcal{E}(J) + \alpha, \quad (3.33)$$

where α and β are Lagrange multipliers. Since $s(x)$ is a strictly concave differentiable function defined on $x \geq 0$, its derivative $s'(x)$ is strictly decreasing on $x \geq 0$, and the inverse function $(s')^{-1}(y)$ exists and is strictly decreasing on the range of the function s' . We are then allowed to put the solution $\tilde{f}_0(J)$ to the variational equation (3.32) in the form

$$\hat{f}_0(\mathcal{E}) = \tilde{f}_0(J(\mathcal{E})) = (s')^{-1}(\beta\mathcal{E} + \alpha). \quad (3.34)$$

The parameter β is positive [CC2010]. To see this, we assume that β were not positive. (i) When $\beta < 0$, from Eq. (3.34), the function $\hat{f}_0(\mathcal{E})$ is strictly increasing with respect to \mathcal{E} , so that the function $\tilde{f}_0(J)$ is strictly increasing with respect to J . (ii) When $\beta = 0$, $\hat{f}_0(\mathcal{E})$ is a constant for the whole \mathcal{E} , so that $\tilde{f}_0(J)$ is a constant for the whole J . In these cases, the integral $\int_L \tilde{f}_0(J) dJ$ diverges, and hence $\tilde{f}_0(J)$ cannot be a probabilistic density function. Hence, parameter β must be positive. In the case $\beta > 0$, $\tilde{f}_0(J)$ can be a probabilistic density function.

Since β is shown to be positive, and since s is strictly concave, a solution (3.34) to the variational equation (3.32) is a stationary solution to the Vlasov equation satisfying $d\hat{f}_0/d\mathcal{E} < 0$ and $d\tilde{f}_0/dJ < 0$.

3.4.3 Formal stability criterion in the most refined form

In this section, we look into the most refined formal stability of the spatially inhomogeneous stationary solution f_0 which is a critical point of the functional (3.31) under the constraint conditions (3.28), (3.29), and (3.30). To start with, we note that $C^n(J) = C^{-n}(J)$. In fact, from $\text{sn}(u, k) = -\text{sn}(-u, k)$ [WW1927] and Eq. (2.51), one has that $\cos q(\theta, J)$ is even with respect to θ , so that $C^n(J)$ is shown to be real from the definition (3.13) and $C^n(J) = C^{-n}(J)$, and further $|C^n(J)|^2 = C^n(J)^2$.

We derive the formal stability criterion for spatially inhomogeneous solutions on the basis of the following claim.

Claim 3 *A solution $\tilde{f}_0(J)$ to the variational equation (3.32) is formally stable, if and only if the second-order variation of the functional $\mathcal{F} = \mathcal{S} - \beta\mathcal{U} - \alpha\mathcal{N}$ is negative definite at \tilde{f}_0 under the constraint of the Casimir invariants. That is, $\delta^2\mathcal{F}[f_0][\delta f, \delta f] < 0$ for any non-zero variation δf*

leaving invariant the functional of the form $Q[f] = \iint_{\mu} Q(f) dqdp$ [Eq. (2.22)] up to first order for any function Q .

To investigate the condition $\delta^2 \mathcal{F} [f_0] [\delta f, \delta f] < 0$, we start by putting the function γ as

$$\gamma(J) = \frac{\beta}{s''(\tilde{f}_0(J))} = \frac{\tilde{f}'_0(J)}{\Omega(J)} = \frac{d\hat{f}_0}{d\mathcal{E}}(\mathcal{E}(J)). \quad (3.35)$$

Then, the second-order variation of \mathcal{F} is described as

$$\begin{aligned} \delta^2 \mathcal{F} [\tilde{f}_0] [\delta \tilde{f}, \delta \tilde{f}] &= \iint_{\mu} \frac{\beta}{\gamma(J)} \delta \tilde{f}(\theta, J)^2 d\theta dJ \\ &+ \beta \left[\iint_{\mu} \cos q(\theta, J) \delta \tilde{f}(\theta, J) d\theta dJ \right]^2 \\ &+ \beta \left[\iint_{\mu} \sin q(\theta, J) \delta \tilde{f}(\theta, J) d\theta dJ \right]^2. \end{aligned} \quad (3.36)$$

On account of the constraints of the Casimir invariants (2.22) up to first order, the perturbation should satisfy the constraint

$$\begin{aligned} Q[f_0 + \delta f] - Q[f_0] &= \iint_{\mu} Q'(f_0(q, p)) \delta f(q, p) dqdp \\ &= \int_L dJ Q'(\tilde{f}_0(J)) \int_{-\pi}^{\pi} \delta \tilde{f}(\theta, J) d\theta \\ &= 0. \end{aligned} \quad (3.37)$$

Since Q is chosen arbitrarily, we can look on $Q'(\tilde{f}_0(J))$ as a function of J (or $\mathcal{E}(J)$) chosen arbitrarily. We are then allowed to restrict perturbations to those satisfying

$$\int_{-\pi}^{\pi} \delta \tilde{f}(\theta, J) d\theta = 0, \quad \forall J. \quad (3.38)$$

We now divide the perturbation $\delta \tilde{f}(\theta, J)$ into even and odd parts with respect to θ ,

$$\delta \tilde{f}(\theta, J) = \delta_e \tilde{f}(\theta, J) + \delta_o \tilde{f}(\theta, J), \quad (3.39)$$

where

$$\begin{aligned} \delta_e \tilde{f}(\theta, J) &= \frac{1}{2} (\delta \tilde{f}(\theta, J) + \delta \tilde{f}(-\theta, J)), \\ \delta_o \tilde{f}(\theta, J) &= \frac{1}{2} (\delta \tilde{f}(\theta, J) - \delta \tilde{f}(-\theta, J)). \end{aligned} \quad (3.40)$$

When $\delta\tilde{f}$ in the functional (3.36) is replaced by (3.39), the functional (3.36) is arranged as

$$\begin{aligned}\delta^2\mathcal{F}[\tilde{f}_0][\delta\tilde{f}, \delta\tilde{f}] &= \iint_{\mu} \frac{\beta}{\gamma(J)} \delta_e\tilde{f}(\theta, J)^2 d\theta dJ + \beta \left[\iint_{\mu} \cos q(\theta, J) \delta_e\tilde{f}(\theta, J) d\theta dJ \right]^2 \\ &\quad + \iint_{\mu} \frac{\beta}{\gamma(J)} \delta_o\tilde{f}(\theta, J)^2 d\theta dJ + \beta \left[\iint_{\mu} \sin q(\theta, J) \delta_o\tilde{f}(\theta, J) d\theta dJ \right]^2 \\ &= \delta^2\mathcal{F}[\tilde{f}_0][\delta_e\tilde{f}, \delta_e\tilde{f}] + \delta^2\mathcal{F}[\tilde{f}_0][\delta_o\tilde{f}, \delta_o\tilde{f}],\end{aligned}\quad (3.41)$$

where we have used the fact that

$$M_x[\delta_o\tilde{f}] = 0, \quad M_y[\delta_e\tilde{f}] = 0, \quad (3.42)$$

which come from the fact that $\cos q(\theta, J)$ (resp. $\sin q(\theta, J)$) is even (resp. odd) with respect to θ on account of Eq. (2.51) (resp. (2.50)). Equation (3.41) means that $\delta_e\tilde{f}$ and $\delta_o\tilde{f}$ are not coupled in Eq. (3.41). As for the second term in the right-hand side of the last equality in Eq. (3.41), we recall that spatially inhomogeneous stationary solutions are already known to be neutrally formally stable against a perturbation $\delta_o\tilde{f}$ whose direction is perpendicular to the direction of the order parameter \vec{M}_0 , as is shown in Ref. [CC2010]. This fact is consistent with the fact that the order parameter may rotate if an arbitrarily small external field is turned on perpendicularly to the order parameter [OY2012]. We do not take into account this rotation as long as we treat a formal stability of the stationary solution f_0 . On account of Eq. (3.42), we are now left with the analysis of, $\delta^2\mathcal{F}[\tilde{f}_0][\delta_e\tilde{f}, \delta_e\tilde{f}]$, the integrals in Eq. (3.41) for the even part $\delta_e\tilde{f}$ whose direction is parallel to the order parameter \vec{M}_0 .

In what follows, we prove the proposition:

Proposition 4 *Let f_0 be a solution to the variational equation (3.32). The inequality*

$$\mathcal{I}[f_0] = D_x(0) > 0 \quad (3.43)$$

is equivalent to the condition

$$\delta^2\mathcal{F}[\tilde{f}_0][\delta_e\tilde{f}, \delta_e\tilde{f}] < 0 \quad (3.44)$$

for any $\delta_e\tilde{f} \neq 0$ under the constraint (3.38). Therefore, the inequality (3.43) is a necessary and sufficient condition for the formal stability of \tilde{f}_0 .

In the situation stated so far, the second order variation (3.36) is put in the form

$$\delta^2\mathcal{F}[\tilde{f}_0][\delta_e\tilde{f}, \delta_e\tilde{f}] = \iint_{\mu} \frac{\beta}{\gamma(J)} \delta_e\tilde{f}(\theta, J)^2 d\theta dJ + \beta \left[\iint_{\mu} \cos q(\theta, J) \delta_e\tilde{f}(\theta, J) d\theta dJ \right]^2. \quad (3.45)$$

We first show that a non-zero $\delta_e\tilde{f}$ satisfying $M_x[\delta_e\tilde{f}] = 0$ does not bring about the formal instability. Indeed, the quadratic form (3.45) becomes

$$\delta^2\mathcal{F}[\tilde{f}_0][\delta_e\tilde{f}, \delta_e\tilde{f}] = \iint_{\mu} \frac{\beta}{\gamma(J)} \delta_e\tilde{f}(\theta, J)^2 d\theta dJ, \quad (3.46)$$

and is negative since $\gamma(J) < 0$ and $\beta > 0$, as was mentioned in Section 3.4.2.

We proceed to perform the stability analysis with the constraint condition

$$M_x [\delta_e \tilde{f}] = \iint_{\mu} \cos q(\theta, J) \delta_e \tilde{f}(\theta, J) d\theta dJ = 1. \quad (3.47)$$

We note that the value of $M_x [\delta_e \tilde{f}]$ can be chosen arbitrary, because this value changes only the scaling of (3.45) and does not change the sign of (3.45). We expand the perturbation $\delta_e \tilde{f}$ into the Fourier series in θ ,

$$\delta_e \tilde{f}(\theta, J) = \sum_{n \neq 0} \hat{f}_n^e(J) e^{in\theta}, \quad \hat{f}_n^e(J) = \hat{f}_{-n}^e(J). \quad (3.48)$$

We note that the 0-th Fourier mode vanishes thanks to the constraint condition (3.38). Substituting (3.48) into the quadratic form (3.45), we obtain the functional in $\{\hat{f}_n^e\}_{n \neq 0}$

$$\begin{aligned} \mathcal{G}_e [\{\hat{f}_n^e\}_{n \neq 0}] &\equiv \frac{1}{2\pi} \delta^2 \mathcal{F} [\tilde{f}_0] [\delta_e \tilde{f}, \delta_e \tilde{f}] \\ &= \sum_{n \neq 0} \int_L \frac{\beta}{\gamma(J)} \hat{f}_n^e(J)^2 dJ + 2\pi\beta \left(\sum_{m \neq 0} \int_L C^m(J') \hat{f}_m^e(J') dJ' \right)^2. \end{aligned} \quad (3.49)$$

We look for a critical point of \mathcal{G}_e under the constraint (3.47) which is rewritten in terms of $\{\hat{f}_n^e\}_{n \neq 0}$ as

$$\mathcal{M}_x [\{\hat{f}_m^e\}_{m \neq 0}] \equiv 2\pi \sum_{m \neq 0} \int_L C^m(J) \hat{f}_m^e(J) dJ = 1. \quad (3.50)$$

The functional $\mathcal{G}_e [\{\hat{f}_m^e\}_{m \neq 0}]$ takes a critical value under the constraint condition (3.50) if

$$\delta_n \mathcal{G}_e [\{\hat{f}_m^e\}_{m \neq 0}] - \eta \delta_n \mathcal{M}_x [\{\hat{f}_m^e\}_{m \neq 0}] = 0, \quad n \in \mathbb{Z} \setminus \{0\}, \quad (3.51)$$

where η is a Lagrange multiplier, and $\delta_n \mathcal{G}_e$ is defined by

$$\begin{aligned} \delta_n \mathcal{G}_e [\{\hat{f}_m^e\}_{m \neq 0}] &\equiv \mathcal{G}_e [\{\hat{f}_m^e + \delta \hat{f}_n^e \delta_{mn}\}_{m \neq 0}] - \mathcal{G}_e [\{\hat{f}_m^e\}_{m \neq 0}] \\ &= 2\beta \int_L \delta \hat{f}_n^e(J) \left[\frac{\hat{f}_n^e(J)}{\gamma(J)} + 2\pi C^n(J) \left(\sum_{m \neq 0} \int_L C^m(J') \hat{f}_m^e(J') dJ' \right) \right] dJ, \end{aligned} \quad (3.52)$$

where δ_{mn} is the Kronecker delta. Hence, Eq. (3.51) results in

$$\hat{f}_n^e(J) = - \left(2\pi \sum_{m \neq 0} \int_L C^m(J') \hat{f}_m^e(J') dJ' \right) C^n(J) \gamma(J) + \frac{\pi\eta}{\beta} C^n(J) \gamma(J) = -\xi C^n(J) \gamma(J), \quad (3.53)$$

for all $n \in \mathbb{Z} \setminus \{0\}$, where we have used Eq. (3.50) and put $\xi \equiv 1 - \pi\eta/\beta$. Substituting Eq. (3.53) into Eq. (3.50), we obtain the value of ξ as

$$\xi = \frac{-1}{2\pi \sum_{m \neq 0} \int_L C^m(J)^2 \gamma(J) dJ}. \quad (3.54)$$

A non-vanishing critical point $\{\hat{f}_n^{\text{e},m}\}_{n \in \mathbb{Z} \setminus \{0\}}$ is therefore given by

$$\hat{f}_n^{\text{e},m}(J) = \frac{C^n(J)\gamma(J)}{2\pi \sum_{m \neq 0} \int_L C^m(J')^2 \gamma(J') dJ'}, \quad n \in \mathbb{Z} \setminus \{0\}. \quad (3.55)$$

Substituting Eq. (3.55) into Eq. (3.49), we obtain

$$\begin{aligned} \mathcal{G}_e \left[\{\hat{f}_n^{\text{e},m}\}_{n \neq 0} \right] &= \frac{\beta}{4\pi^2 \sum_{m \neq 0} \int_L C^m(J)^2 \gamma(J) dJ} + \frac{\beta}{2\pi} \\ &= \frac{\beta}{4\pi^2 \sum_{m \neq 0} \int_L C^m(J)^2 \gamma(J) dJ} \times \left[1 + 2\pi \sum_{l \neq 0} \int_L \frac{\tilde{f}'_0(J)}{\Omega(J)} C^l(J)^2 dJ \right], \end{aligned} \quad (3.56)$$

where we have used Eq. (3.35).

Since $\gamma(J) < 0$, and since $C^n(J) \neq 0$ for some J and $n \in \mathbb{Z} \setminus \{0\}$, we have

$$\sum_{m \neq 0} \int_L C^m(J)^2 \gamma(J) dJ < 0. \quad (3.57)$$

It then follows, from Eq. (3.56) along with Eq. (3.57) and the positivity of β which has been shown at the end of Section 3.4.2, that the quadratic form (3.49) is negative definite if and only if the inequality

$$D_x(0) = 1 + 2\pi \sum_{l \neq 0} \int_L \frac{\tilde{f}'_0(J)}{\Omega(J)} C^l(J)^2 dJ > 0 \quad (3.58)$$

is satisfied. We hence conclude that the inequality (3.43) is a necessary and sufficient condition for formal stability. Once the criterion (3.43) is obtained, we no longer have to seek an infinite number of Lagrange multipliers to get the most refined formal stability criterion given in Ref. [CC2010]. The formal stability criterion (3.43) is stronger than the condition that $\tilde{f}_0(J)$ is spectrally stable in the sense that the equality in Eq. (3.12) is not allowed.

Remark. We have shown that the stability of f_0 is determined by the sign of $\mathcal{I}[f_0] = D_x(0)$. Further the value of the positive $\mathcal{I}[f_0]$ is thought to express a strength of stability of f_0 since the zero-field isolated-susceptibility χ is derived as

$$\chi = \frac{1 - D_x(0)}{D_x(0)} = \frac{1 - \mathcal{I}[f_0]}{\mathcal{I}[f_0]}, \quad (3.59)$$

with the linear response theory based on the Vlasov equation [OY2012]. Equation (3.59) implies that stability of a stationary state f_0 becomes stronger as $\mathcal{I}[f_0]$ becomes larger, since $\mathcal{I}[f_0] = D_x(0) \leq 1$. The last inequality is derived as follows. As we mentioned in Section 3.4.1, the function $D_x(i\omega_i)$ is strictly increasing and continuous with respect to $\omega_i \geq 0$, and $D_x(i\omega_i) \rightarrow 1$, as $\omega_i \rightarrow \infty$.

3.4.4 Observation of the criteria

Let us observe what kinds of stationary states are likely to be stable through the stability analysis for a family of the stationary waterbag distributions [BOY2010],

$$\begin{aligned} f_{\text{wb}}(q, p) &= \eta_0 \Theta(\mathcal{E}^* - \mathcal{E}(q, p)), \\ \mathcal{E}(q, p) &= \frac{p^2}{2} - M_0 \cos q, \end{aligned} \quad (3.60)$$

where Θ is the Heaviside step function. Let us put $k^* = \sqrt{\frac{\mathcal{E}^* + M_0}{2M_0}}$. For each fixed M_0 , the two parameters η_0 and \mathcal{E}^* are determined by the normalization condition

$$\begin{aligned} 1 &= \iint_{\mu} f_{\text{wb}}(q, p) dq dp \\ &= \begin{cases} 16\eta_0 \sqrt{M_0} (E(k^*) - (1 - k^{*2})K(k^*)), & k^* < 1, \\ 16\eta_0 \sqrt{M_0} k^* E(1/k^*), & k^* > 1, \end{cases} \end{aligned} \quad (3.61)$$

and the self-consistent equation,

$$\begin{aligned} M_0 &= \iint_{\mu} \cos q f_{\text{wb}}(q, p) dq dp \\ &= \begin{cases} 1 - \frac{2(2 - k^{*2})E(k^*) - (2 - 2k^{*2})K(k^*)}{3(E(k^*) - (1 - k^{*2})K(k^*))}, & k^* < 1, \\ \frac{2k^{*2} - 1}{3} - \frac{2k^{*2} - 2}{3} \frac{K(1/k^*)}{E(1/k^*)}, & k^* > 1. \end{cases} \end{aligned} \quad (3.62)$$

For the waterbag distribution (3.60), we are able to compute $\mathcal{I}[f_{\text{wb}}]$ explicitly by using equations

$$\frac{1}{p} \frac{\partial f_{\text{wb}}}{\partial p}(q, p) = \frac{d\widehat{f_{\text{wb}}}}{d\mathcal{E}}(\mathcal{E}(q, p)) = -\eta_0 \delta(\mathcal{E}^* - \mathcal{E}(q, p)), \quad (3.63)$$

and

$$\frac{d\bar{f}_0}{dk}(k) = 4M_0 k \frac{d\widehat{f}_0}{d\mathcal{E}}(\mathcal{E}(k)) = -4M_0 k \eta_0 \delta(\mathcal{E}^* - \mathcal{E}(k)), \quad (3.64)$$

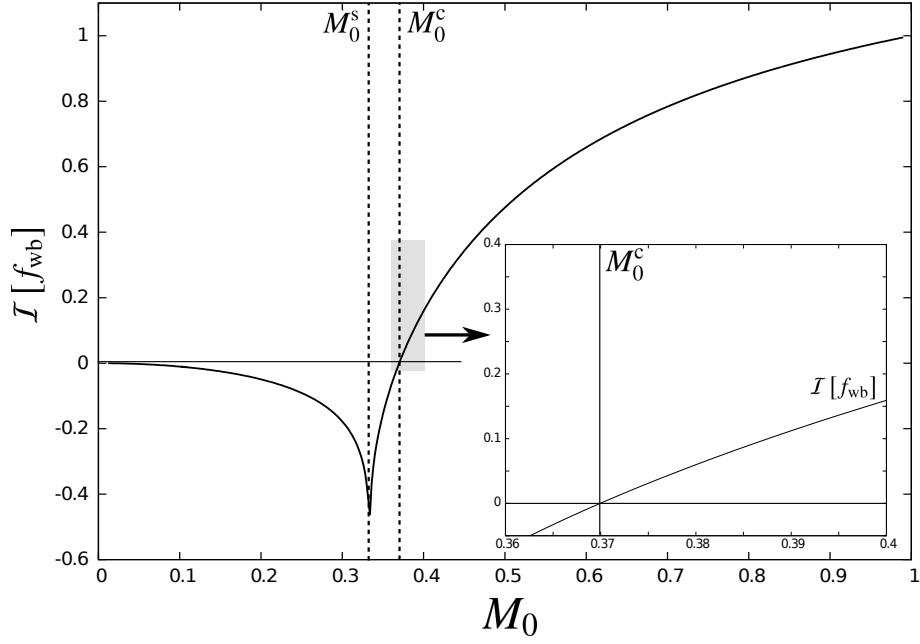


Figure 3.1: Plot of $\mathcal{I}[f_{\text{wb}}]$ as a function of M_0 : $\mathcal{I}[f_{\text{wb}}] > 0$ for $M_0 > M_0^c$. The critical value $M_0^c \simeq 0.369942$. The edge of the waterbag $\mathcal{E}(q, p) = \mathcal{E}^*$ coincides with the separatrix when $M_0 = M_0^s \simeq 0.33$.

and by using Eq. (3.27). Then, $\mathcal{I}[f_{\text{wb}}]$ is written as

$$\mathcal{I}[f_{\text{wb}}] = \begin{cases} 1 + \frac{(8k^{*2} - 4)E(k^*) + (1 - 4k^{*2})K(k^*)}{12M_0[E(k^*) - (1 - k^{*2})K(k^*)]} + \frac{(2E(k^*) - K(k^*))^2}{4M_0K(k^*)[E(k^*) - (1 - k^{*2})K(k^*)]}, & k^* < 1, \\ 1 + \frac{(8k^{*4} - 4k^{*2})E(1/k^*) - (8k^{*4} - 8k^{*2} + 3)K(1/k^*)}{12M_0k^{*2}E(1/k^*)} + \frac{(2k^{*2}E(1/k^*) + (1 - 2k^{*2})K(1/k^*))^2}{4M_0k^*K(1/k^*)E(1/k^*)}, & k^* > 1. \end{cases} \quad (3.65)$$

Since \mathcal{E}^* and k^* is determined with M_0 , then $\mathcal{I}[f_{\text{wb}}]$ in Eq. (3.65) can be looked on as a function of M_0 and it is plotted in Fig. 3.1. According to this graph, the waterbag f_{wb} is formally (resp. spectrally) stable when $M_0 > M_0^c \simeq 0.369942$ (resp. when $M_0 \geq M_0^c$). The critical value $M_0^c \simeq 0.369942$ is obtained by solving the self-consistent equation (3.62) and $\mathcal{I}[f_{\text{wb}}] = 0$ simultaneously, and it is close to the estimation $M_0^c \simeq 0.37$ in Ref. [BOY2010]. The waterbag distribution with large M_0 tends to be stable, and the stability of it tends to be strong, since $\mathcal{I}[f_{\text{wb}}]$ is monotonically increasing with respect to M_0 , when $M_0 > M_0^s \simeq 0.33$. We illustrate it in Fig. 3.2. The waterbag distributions illustrated in panels (a) or (b) are unstable, and one illustrated in panel (c) is stable.

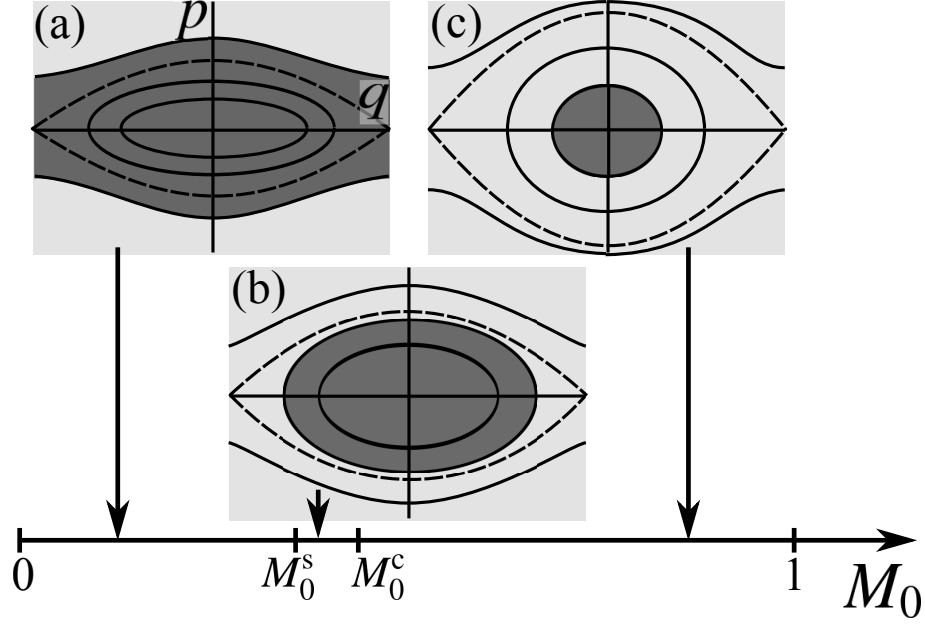


Figure 3.2: Gray rectangles are μ spaces for each M_0 . The curves in μ spaces are iso- \mathcal{E} lines, and the broken curves are separatrices. On the dark gray region in each μ space, the waterbag distribution takes non-zero value, η_0 .

3.5 Comparing with the canonical formal stability criterion

Let us compare the formal stability criterion (3.43), $\mathcal{I}[f_0] = D_x(0) > 0$, with the *canonical formal stability* criterion given in Ref. [CC2010]. We start with a brief review of the canonical formal stability.

3.5.1 The canonical formal stability

Claim 5 ([CC2010]) *A solution f_0 to the variational equation (3.32) is called canonically formally stable against any perturbation $\delta_e f$ whose direction is parallel to the order parameter $\vec{M}_0 = (M_0, 0)^T$, if and only if the second order variation of the functional $\mathcal{F} = \mathcal{S} - \beta\mathcal{E} - \alpha\mathcal{N}$ at f_0 , $\delta^2\mathcal{F}[f_0]$, subject to the normalization condition is negative definite, i.e.,*

$$\delta^2\mathcal{F}[f_0][\delta_e f, \delta_e f] < 0, \quad (3.66)$$

for all $\delta_e f \neq 0$ satisfying

$$\iint_{\mu} \delta_e f(q, p) dq dp = 0. \quad (3.67)$$

In particular, for the HMF model, the spatially inhomogeneous solution $f_0(q, p)$ is canonically formally stable if and only if

$$\mathcal{I}_C[f_0] \equiv 1 + \int_{-\pi}^{\pi} dq \cos^2 q \int_{-\infty}^{\infty} \frac{1}{p} \frac{\partial f_0}{\partial p}(q, p) dp - \frac{\left(\int_{-\pi}^{\pi} dq \cos q \int_{-\infty}^{\infty} \frac{1}{p} \frac{\partial f_0}{\partial p}(q, p) dp \right)^2}{\int_{-\pi}^{\pi} dq \int_{-\infty}^{\infty} \frac{1}{p} \frac{\partial f_0}{\partial p}(q, p) dp} > 0. \quad (3.68)$$

Satisfying the inequality (3.68) is sufficient but not necessary for the formal stability. We will show the existence of stationary solutions f_0 which are not canonically formally stable, but formally stable in the most refined sense.

3.5.2 Example: Family of distributions having metastable states

In this subsection, we prove the following proposition:

Proposition 6 *Let D be a subset of \mathbb{R}^n . Assume that a family of smooth stationary solutions $\mathcal{X} = \{f_0(q, p; M_0, \lambda) \mid \lambda \in D\}$, which are parametrized with the order parameter $M_0 = M_x[f_0]$ and a set of macroscopic quantities $\lambda = (\lambda_1, \lambda_2, \dots, \lambda_n) \in D$, such that there exists $f_0^b(q, p) = f_0(q, p; M_0^b, \lambda^b) \in \mathcal{X}$ satisfying $\mathcal{I}[f_0^b] = 0$ and $M[f_0^b] > 0$. Moreover, assume that both $\mathcal{I}[f_0](M_0, \lambda)$ and $\mathcal{I}_C[f_0](M_0, \lambda)$ depend on M_0 and λ continuously. Then, there are stationary solutions $f_0 \in \mathcal{X}$ which do not satisfy the canonical formal stability criterion, $\mathcal{I}_C[f_0](M_0, \lambda) > 0$ [Eq. (3.68)], but do satisfy the formal stability criterion, $\mathcal{I}[f_0](M_0, \lambda) = D_x(0) > 0$ [Eq. (3.43)].*

Remark. If the system has a first-order phase transition and a two-phase coexistence region in a parameter space (M_0, λ) , then we can take a family \mathcal{X} of stationary solutions satisfying assumptions in Prop. 6. An example of such a family \mathcal{X} is known in Lynden-Bell's distributions (or Fermi-Dirac type distributions) [Lyn1967]. Within the Lynden-Bell's statistical mechanics with two-valued waterbag initial conditions, single-body distributions are parametrized with the order parameter in stationary states M_0 , the energy U , and the parameter M_{wb} describing to what extent particles spread on the μ space before violent relaxation occurs. In this case, one has $n = 2$ and $(\lambda_1, \lambda_2) = (U, M_1)$ [AFRY2007, SCD2011, OY2011]. A schematic picture of the phase diagram (M_0, U, M_{wb}) is exhibited in Fig. 3.3. On the three-dimensional parameter space, one can observe a first-order phase transition, a tricritical point, and a two-phase coexistence region.

We will omit the parameters (M_0, λ) from the description of f_0 , $\mathcal{I}[f_0]$ and $\mathcal{I}_C[f_0]$ as long as no confusion arises. To prove the proposition, we first rewrite the third term of the right-hand side of (3.68) in terms of the angle-action coordinates,

$$\frac{\left(\int_{-\pi}^{\pi} dq \cos q \int_{-\infty}^{\infty} \frac{1}{p} \frac{\partial f_0}{\partial p}(q, p) dp \right)^2}{\int_{-\pi}^{\pi} dq \int_{-\infty}^{\infty} \frac{1}{p} \frac{\partial f_0}{\partial p}(q, p) dp} = 2\pi \frac{\left(\int_L \frac{\tilde{f}'_0(J)}{\Omega(J)} C^0(J) dJ \right)^2}{\int_L \frac{\tilde{f}'_0(J)}{\Omega(J)} dJ}. \quad (3.69)$$

The difference between $\mathcal{I}[f_0]$ and $\mathcal{I}_C[f_0]$ is calculated as

$$\begin{aligned}\mathcal{I}[f_0] - \mathcal{I}_C[f_0] &= -2\pi \int_L \frac{\tilde{f}_0'(J)}{\Omega(J)} C^0(J)^2 dJ + 2\pi \frac{\left(\int_L \frac{\tilde{f}_0'(J)}{\Omega(J)} C^0(J) dJ \right)^2}{\int_L \frac{\tilde{f}_0'(J)}{\Omega(J)} dJ} \\ &= -2\pi \int_L \frac{\tilde{f}_0'(J')}{\Omega(J')} dJ' \left[\int_L C^0(J)^2 P(J) dJ - \left(\int_L C^0(J) P(J) dJ \right)^2 \right],\end{aligned}\quad (3.70)$$

where $P(J)$ is defined to be

$$P(J) \equiv \frac{1}{\int_L \frac{\tilde{f}_0'(J')}{\Omega(J')} dJ'} \frac{\tilde{f}_0'(J)}{\Omega(J)} \geq 0. \quad (3.71)$$

We note that the inequality,

$$\int_L C^0(J)^2 P(J) dJ - \left(\int_L C^0(J) P(J) dJ \right)^2 \geq 0, \quad (3.72)$$

is satisfied for any f_0 . In fact, on account of

$$\int_L P(J) dJ = 1, \quad (3.73)$$

we obtain the equation,

$$\begin{aligned}&\int_L C^0(J)^2 P(J) dJ - \left(\int_L C^0(J) P(J) dJ \right)^2 \\ &= \int_L \left[C^0(J) - \int_L C^0(J') P(J') dJ' \right]^2 P(J) dJ,\end{aligned}\quad (3.74)$$

which implies Eq. (3.72). If the equality holds in Eq. (3.72), Eq. (3.74) results in

$$C^0(J) = \int_L C^0(J') P(J') dJ' = \text{Constant}, \quad \forall J. \quad (3.75)$$

However, this equality cannot be realized for any smooth spatially inhomogeneous solution, so that Eq. (3.72) should be

$$\int_L C^0(J)^2 P(J) dJ - \left(\int_L C^0(J) P(J) dJ \right)^2 > 0. \quad (3.76)$$

Equation (3.70) with $\gamma(J) < 0$ and this inequality are put together to provide

$$\mathcal{I}[f_0] > \mathcal{I}_C[f_0] \quad (3.77)$$

for any smooth spatially inhomogeneous stationary solution f_0 . This implies the known inclusion relation [CC2010]

$$\begin{aligned} & \{\text{canonically formally stable states}\} \\ & \cap \\ & \{\text{formally stable states}\}. \end{aligned} \quad (3.78)$$

We show that there is a solution which is formally stable but not canonically formally stable. From the assumption in Prop. 6,

$$\mathcal{I}[f_0^b] = 0. \quad (3.79)$$

If one could decide the formal stability of a stationary solution correctly by using the canonical formal stability criterion (3.68) near the stationary solution f_0^b , the equation

$$\mathcal{I}_c[f_0^b] = 0 \quad (3.80)$$

would be satisfied as well, since $\mathcal{I}_c[f_0]$ depends on the parameters continuously. However, we have proved the inequality (3.77), so that Eqs. (3.79) and (3.80) do not hold simultaneously. Then, the inequality

$$\mathcal{I}_c[f_0^b] < \mathcal{I}[f_0^b] = 0 \quad (3.81)$$

should be satisfied. From Eqs. (3.77) and (3.81), it follows that there exists f_0 such that

$$\mathcal{I}_c[f_0] \leq 0, \quad \mathcal{I}[f_0] > 0. \quad (3.82)$$

This implies that there is a solution which is formally stable, but not canonically formally stable.

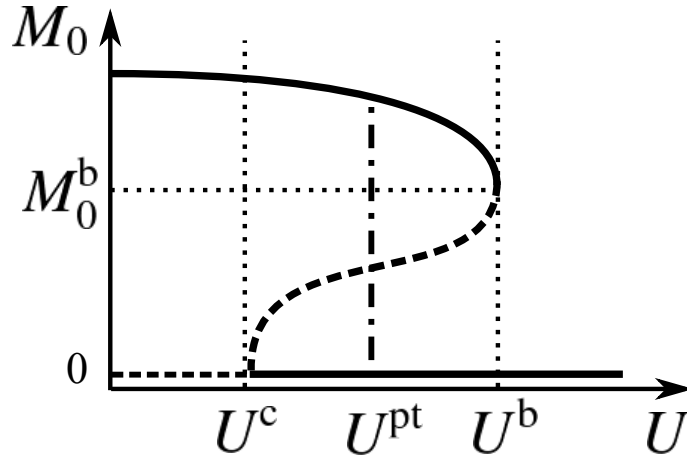


Figure 3.3: Schematic picture of the phase diagram on (M_0, U) for some fixed M_{wb} [AFRY2007]. The solid curve represents the stable or metastable states which are realized as the local maximum points of the entropy. The broken curve represents the unstable states which are realized as the local minimum points of the entropy. These two curves meet at (M_0^b, U^b) . A region between U^c and U^b is called the two-phase coexistence region, and the first-order phase transition occurs at U^{pt} .

3.6 Summary and discussion

We have worked out the spectral and formal stability criteria for spatially inhomogeneous stationary solutions to the Vlasov equation for the HMF model. These criteria are stated in the form of necessary and sufficient conditions (see Props. 2 and 4). We stress that the assumptions for deriving the spectral stability criterion are satisfied by solutions to the variational equation (3.32). Our criterion avoids the problem of finding an infinite number of Lagrange multipliers which are required in the previously obtained criterion [CC2010]. We note that the formal stability criterion in Prop. 4 is stated in the form modified from the original one in Ref. [HMRW1985], since the perturbation $\delta_o \tilde{f}$ perpendicular to the order parameter \vec{M}_0 with $M_y[\delta_o \tilde{f}] \neq 0$ brings about the neutral formal stability, and since the set of neutrally formally stable solutions is defined so as not to be included in the set of formally stable ones by [HMRW1985].

We have interpreted the value of $\mathcal{I}[f_0] = D_x(0)$ as the strength of stability of the stable solutions. Further, we have observed that the stationary state with high density almost harmonic orbits tends to be stable, and its stability gets to be stronger as M_0 gets large.

We have shown that stability of some solutions in the family of stationary solutions having two-phase coexistence region in the phase diagram cannot be judged correctly by using the canonical formal stability criterion (see Prop. 6). A family of the Lynden-Bell's distributions is a family to which Prop. 6 is applied.

So far we have analyzed stability criteria for the HMF model without external fields. The present methods can be applied for the HMF model with non-zero external field, if the Hamiltonian takes the form

$$H_N = \sum_{i=1}^N \frac{p_i^2}{2} + \frac{1}{2N} \sum_{i,j=1}^N (1 - \cos(q_i - q_j)) - h \sum_{i=1}^N \cos q_i. \quad (3.83)$$

All we have to do is to modify the single-body energy (3.9) by adding to the potential $-M_0 \cos q$ the term $-h \cos q$ coming from external field. Then, we can make a similar discussion by using the angle-action coordinates. In this case, the rotational symmetry is broken, so that $D_y(0) \neq 0$. Hence, the spectral and the formal stability criteria become

$$D_x(0) \geq 0, \quad D_y(0) \geq 0, \quad (3.84)$$

and

$$D_x(0) > 0, \quad D_y(0) > 0, \quad (3.85)$$

respectively, and further the value of $D_y(0)$ is computed as $D_y(0) = h/(M_0 + h)$ by using the same procedure as in Eq. (3.25). In this case, the definition of formal stability is the same as one defined in Ref. [HMRW1985], so that we can refer to the linear stability condition. Equation (3.84) is a necessary condition for the linear stability of the spatially inhomogeneous solution, and Eq. (3.85) is a sufficient condition of it. In fact, linearly stable states are spectrally stable states, and formally stable states are linearly stable states. This statement can be shown as follows [HMRW1985]:

- If f_0 is spectrally unstable, f_0 is not linearly stable, because there exists an unstable eigenmode. By taking its contraposition, the former part is shown.

- If f_0 is formally stable, the quadratic form $\delta^2 \mathcal{F}[f_0][\delta f, \delta f]$ given by Eq. (3.36) is negative definite. Then, we can define a norm in Eq. (3.3) as $\|\delta f\| \equiv \sqrt{-\delta^2 \mathcal{F}[f_0][\delta f, \delta f]}$. This norm is preserved with the linearized Vlasov equation, and f_0 is shown to be linearly stable.

This discussion breaks down for the spatially inhomogeneous states in the HMF model without external field.

The stability analysis performed in the present chapter is applicable to the generalized HMF model (2.72) with the uniform external field h . We consider the stationary state $f_0(q, p)$ does not depend on the lattice point r and does satisfy the assumptions in Claim 3. Then, the stationary state $f_0(q, p)$ also satisfies the assumptions in Prop. 2. The spectral and formal stability criteria for such a stationary state $f_0(q, p)$ are

$$D_x^n(0) \geq 0, \quad D_y^n(0) \geq 0, \quad \forall n \in \mathbb{Z}, \quad (3.86)$$

and

$$D_x^n(0) > 0, \quad D_y^n(0) > 0, \quad \forall n \in \mathbb{Z}, \quad (3.87)$$

respectively. By using Eqs. (2.70) and (2.82), we obtain the explicit forms of $D_x^n(0)$ and $D_y^n(0)$ as

$$\begin{aligned} D_x^n(0) &= 1 + 2\pi K_n \sum_{m \in \mathbb{Z} \setminus \{0\}} \int_L \frac{f'_0(J)}{\Omega(J)} |C^m(J)|^2 dJ, \\ D_y^n(0) &= 1 + 2\pi K_n \sum_{m \in \mathbb{Z} \setminus \{0\}} \int_L \frac{f'_0(J)}{\Omega(J)} |S^m(J)|^2 dJ, \end{aligned} \quad (3.88)$$

respectively. Since the site-site interaction $K(r)$ is assumed to satisfy $K(r) = K(-r)$ and $K(r) \geq 0$ for all $r \in (-1/2, 1/2]$ in this thesis (see Section 2.5) it is shown the inequality

$$|K_n| \leq K_0 = 1, \quad (3.89)$$

for all $n \in \mathbb{Z} \setminus \{0\}$. Since all integrals included in Eq. (3.88) are negative, we can reduce the criteria (3.86) and (3.87) to

$$D_x^0(0) \geq 0, \quad D_y^0(0) \geq 0, \quad (3.90)$$

and

$$D_x^0(0) > 0, \quad D_y^0(0) > 0, \quad (3.91)$$

respectively.

Our procedure to look into the formal stability of the HMF model may be formally generalized to other models by using the biorthogonal functions and the Kalnajs' matrix form, which have been used in the astrophysics [BT2008, BOY2011, Kal1971]. However, there are difficulties in extending our result for the HMF model to that for general models. For instance, finding an appropriate biorthogonal system and analyzing the Kalnajs' matrix form are hard tasks. In fact, the dispersion function is not a complex-valued function but a linear operator or a matrix. Hence, the formal stability criterion should be described in the form of positive definiteness of matrices or linear operators. If this matrix is a diagonal matrix or a block diagonal matrix with small blocks, we may get the formal stability criterion as for the HMF model for each diagonal element or each block.

Chapter 4

Linear response theory in quasi-stationary states

4.1 Introduction

The statistical mechanics for QSSs has been considered without operations of the external fields until recent studies [PGN2012, OY2012, Cha2013]. It is important to understand response to external fields or external forces which represent operations, for instance adiabatic compression for gas confined in a box, and exerting external magnetic field for a magnetic material to construct thermodynamics in QSSs. We stress that we must describe such operations and theory of response to the external fields in the context of the Vlasov dynamics, since QSSs are recognized as stable stationary solutions to the Vlasov equation as we mentioned in previous chapters. Another important topic in investigating the linear response is that one can obtain non-equilibrium dynamics in unforced systems by exerting weak probe fields and measuring linear response to these fields. Such a response theory may be then compatible with an experimental setting.

Writing the linear response theory based on the Vlasov equation has an advantage against the Kubo formula for classical systems based on the Liouville equation. The Kubo formula requires to solve equations of motion for an N -body Hamiltonian system [Kub1957, KTH1985], but an N -body system is non-integrable in general. On the other hand, the Vlasov equation is described by a single-body Hamiltonian, and the system is integrable when spatial dimension is one and a considering state is stationary.

The linear response theory in the Vlasov equation has been also proposed by Patelli et al. [PGN2012]. We clarify advantages of the present chapter against the previous work:

- They assume that conjugate variables of external field depend on position variables only, but we do not require this assumption in a general theory.
- They do not deal with response around spatially inhomogeneous QSSs, but the present theory includes both homogeneous and inhomogeneous cases.
- The present chapter investigates the Curie-Weiss law like behavior of zero-field susceptibility for some QSSs.
- We use the linear response theory to extract non-equilibrium dynamics in spatially inhomogeneous states of the unforced HMF model. We try to probe the Landau poles by resonance

absorption instead of directly solving the dispersion relation.

This chapter is organized as follows. We propose the explicit but formal linear response theory based on the Vlasov equation for spatially periodic one-dimensional systems in Section 4.2. The linear response is described by two families of functions, and concrete forms of the functions are given in Section 4.3 both for homogeneous and for the inhomogeneous cases. The theory is applied for the HMF model in Section 4.4, and is numerically examined for the homogeneous case in Section 4.5 and for the inhomogeneous case in Section 4.6. We discuss the critical exponent for the isolated susceptibility in the ordered phase in Section 4.7. Section 4.8 is devoted to a summary and discussions.

4.2 Linear response theory for the Vlasov equation in general framework

We consider a spatially periodic one-dimensional Hamiltonian system consisting of N particles and add a small external field to the system. Let the Hamiltonian of this system be

$$\begin{aligned} H_N(q_1, \dots, q_N, p_1, \dots, p_N, t) \\ = \sum_{i=1}^N \frac{p_i^2}{2} + \frac{1}{N} \sum_{i < j} V(q_i - q_j) + \sum_{i=1}^N H_1(q_i, p_i, t). \end{aligned} \quad (4.1)$$

The position q_i is defined on a circle and its domain is $q_i \in [-\pi, \pi)$, and $p_i \in \mathbb{R}$ is the conjugate momentum. The terms of H_1 represent energy added by the time-dependent external field. In the large N limit, temporal evolution of the system is described by the single-body distribution function f obeying the Vlasov equation,

$$\frac{\partial f}{\partial t} + \{\mathcal{H}[f], f\} = 0. \quad (4.2)$$

The single-body Hamiltonian is expressed by [PGN2012]

$$\mathcal{H}[f](q, p, t) = \mathcal{H}_0[f](q, p, t) + H_1(q, p, t), \quad (4.3)$$

where

$$\mathcal{H}_0[f](q, p, t) = \frac{p^2}{2} + \mathcal{V}[f](q, t), \quad (4.4)$$

$$\mathcal{V}[f](q, t) = \iint_{\mu} V(q - q') f(q', p, t) dq' dp. \quad (4.5)$$

4.2.1 Implicit linear response

For investigating linear response around a stationary state, we set $H_1 = 0$ for $t < 0$ and add the small external field at $t = 0$. Before adding the external field, the Vlasov equation is written as

$$\frac{\partial f}{\partial t} + \{\mathcal{H}_0[f], f\} = 0. \quad (4.6)$$

Let $f_0(q, p)$ be a stationary solution to the Vlasov equation with $H_1 = 0$, and hence satisfy

$$\{\mathcal{H}_0[f_0], f_0\} = 0 \quad (4.7)$$

at any time t . The added small external field represented by H_1 induces a small change of the distribution function from f_0 , and we write the modified distribution function as

$$f(q, p, t) = f_0(q, p) + f_1(q, p, t). \quad (4.8)$$

We assume that amplitude of f_1 is the same order with or smaller than H_1 . Substituting Eq. (4.8) into the Vlasov equation (4.2), we obtain the linearized Vlasov equation

$$\frac{\partial f_1}{\partial t} = -\{\mathcal{H}_0[f_0], f_1\} - \{\mathcal{V}[f_1] + H_1, f_0\}, \quad (4.9)$$

where the higher order term $\{\mathcal{V}[f_1] + H_1, f_1\}$ was omitted. Introducing the operator \mathcal{L}_0 defined by

$$\mathcal{L}_0 f_1 = -\{\mathcal{H}_0[f_0], f_1\}, \quad (4.10)$$

the linearized Vlasov equation is rewritten as

$$\frac{\partial f_1}{\partial t} = \mathcal{L}_0 f_1 - \{\mathcal{V}[f_1] + H_1, f_0\}. \quad (4.11)$$

The formal solution to Eq. (4.11) is, noting that $f_1 = 0$ for $t < 0$,

$$f_1(q, p, t) = - \int_0^t e^{(t-s)\mathcal{L}_0} \{\mathcal{V}[f_1](s) + H_1(s), f_0\} ds, \quad (4.12)$$

where we omitted arguments in the right-hand side except for the time.

Let us introduce an observable B which is a smooth function on μ space, the (q, p) plane. Response to the small external field is observed by the expected value of B with respect to f_1 defined by

$$\langle B \rangle_1(t) = \iint_{\mu} B(q, p) f_1(q, p, t) dq dp. \quad (4.13)$$

Substituting the formal solution (4.12) into Eq. (4.13), we have

$$\langle B \rangle_1(t) = - \int_0^t ds \iint_{\mu} B_{t-s}(q, p) \{\mathcal{V}[f_1](s) + H_1(s), f_0\} dq dp. \quad (4.14)$$

The new function $B_t(q, p)$ is defined by

$$B_t(q, p) = (B \circ \phi_0^t)(q, p), \quad (4.15)$$

where ϕ_0^t is the Hamiltonian flow induced by the Hamiltonian $\mathcal{H}_0[f_0]$. See Appendix C.1 for deriving Eq. (4.14).

The expression (4.14) is the linear response of B for the small external field, but is implicit since the unknown function f_1 appears both in the left- and right-hand sides. We will write $\mathcal{V}[f_1]$ by known quantities, and give an explicit linear response in the next section.

4.2.2 Explicit linear response

Thanks to the periodic boundary condition, any functions of q are periodic, and hence can be expanded in the Fourier series as

$$f_1(q, p, t) = \sum_{k \in \mathbb{Z}} f_{1,k}(p, t) e^{ikq} \quad (4.16)$$

and

$$V(q) = \sum_{k \in \mathbb{Z}} V_k e^{ikq}. \quad (4.17)$$

Substituting Eqs. (4.16) and (4.17) into Eq. (4.5), we have

$$\mathcal{V}[f_1](q, t) = 2\pi \sum_{k \in \mathbb{Z}} V_k e^{ikq} \rho_{1,k}(t), \quad (4.18)$$

where

$$\rho_{1,k}(t) = \frac{1}{2\pi} \iint_{\mu} e^{-ikq} f_1(q, p, t) dq dp = \frac{1}{2\pi} \langle e^{-ikq} \rangle_1 \quad (4.19)$$

is the Fourier transform of the density function ρ_1 defined by

$$\rho_1(q, t) = \int f_1(q, p, t) dp. \quad (4.20)$$

We substitute Eq. (4.18) into Eq. (4.14), and choose B as e^{-ikq} to obtain an equation for $\rho_{1,k}(t)$. For later convenience, we write the exponential factor as a function on μ space as

$$E^k(q, p) = e^{-ikq}, \quad (4.21)$$

where E^k has the argument p but does not depend on p . We then obtain

$$2\pi \rho_{1,k}(t) = - \iint_{\mu} dq dp \int_0^t E_{t-s}^k \left\{ 2\pi \sum_{l \in \mathbb{Z}} V_l E^{-l} \rho_{1,l}(s) + H_1(s), f_0 \right\} ds. \quad (4.22)$$

To treat the convolution with respect to time in Eq. (4.22), we perform the Laplace transform, which is defined by

$$\tilde{\varphi}(\omega) = \int_0^\infty \varphi(t) e^{i\omega t} dt, \quad (\text{Im } \omega > 0) \quad (4.23)$$

for a function $\varphi(t)$. The condition $\text{Im } \omega > 0$ ensures convergence of the Laplace transform for non-diverging $\varphi(t)$. The equation for $\rho_{1,k}$, Eq. (4.22), is then transformed to

$$\tilde{\rho}_{1,k}(\omega) = \sum_{l \in \mathbb{Z}} \tilde{F}_{kl}(\omega) \tilde{\rho}_{1,l}(\omega) + \tilde{G}_k(\omega), \quad (4.24)$$

where

$$\tilde{F}_{kl}(\omega) = -V_l \iint_{\mu} \tilde{E}_\omega^k(q, p) \{E^{-l}, f_0\} dq dp \quad (4.25)$$

and

$$\tilde{G}_k(\omega) = -\frac{1}{2\pi} \iint_{\mu} \tilde{E}_{\omega}^k(q, p) \{\tilde{H}_1(\omega), f_0\} dq dp. \quad (4.26)$$

Let us introduce the vectors $\tilde{\rho}_1(\omega) = (\tilde{\rho}_{1,k}(\omega))$, $\tilde{G}(\omega) = (\tilde{G}_k(\omega))$ and the matrix $F(\omega) = (F_{kl}(\omega))$. Equation (4.24) is, thus, formally written in a simple form as

$$\tilde{\rho}_1(\omega) = \tilde{F}(\omega) \tilde{\rho}_1(\omega) + \tilde{G}(\omega), \quad (4.27)$$

and the formal solution is

$$\tilde{\rho}_1(\omega) = (I - \tilde{F}(\omega))^{-1} \tilde{G}(\omega), \quad (4.28)$$

where I is the identity matrix.

Let us come back to rewrite the implicit linear response (4.14) into an explicit linear response. The Laplace transform of $\mathcal{V}[f_1]$ is, from Eq. (4.18),

$$\begin{aligned} \tilde{\mathcal{V}}[f_1](q, \omega) &= 2\pi \sum_{k \in \mathbb{Z}} V_k e^{ikq} \tilde{\rho}_{1,k}(\omega) = v \cdot \tilde{\rho}_1(\omega) \\ &= v(q) \cdot (I - \tilde{F}(\omega))^{-1} \tilde{G}(\omega) \end{aligned} \quad (4.29)$$

where the vector $v(q)$ is defined by $v(q) = (2\pi V_k e^{ikq})$ and $v \cdot \tilde{\rho}_1$ represents the Euclidean inner product between v and $\tilde{\rho}_1$. Finally, the Laplace transformed linear response is expressed in the form

$$\langle \tilde{B} \rangle_1(\omega) = - \iint_{\mu} \tilde{B}_{\omega} \{v \cdot (I - \tilde{F}(\omega))^{-1} \tilde{G}(\omega) + \tilde{H}_1(\omega), f_0\} dq dp. \quad (4.30)$$

We give some remarks on Eq. (4.30). (i) The right-hand side of Eq. (4.30) does not include f_1 , and consists of the given external field H_1 and quantities computed from f_0 . (ii) The external field H_1 and the observable B are functions of both q and p , while the previous work assumed that they are functions of q only [PGN2012]. (iii) The stationary solution f_0 is not assumed as spatially homogeneous. (iv) An important step to compute the right-hand side of Eq. (4.30) is to obtain \tilde{E}_{ω}^k , which gives F and G functions. (v) The expression (4.30) is explicit but formal in general, since the size of matrix F may be infinite.

We also remark that the relation

$$\iint_{\mu} \phi \{\psi, f_0\} dq dp = \iint_{\mu} \{\phi, \psi\} f_0 dq dp = \langle \{\phi, \psi\} \rangle_0 \quad (4.31)$$

can be shown for smooth functions ϕ and ψ when f_0 is a rapidly decreasing function of p in the large $|p|$ by using integration by parts and the periodic boundary condition for q . Here $\langle B \rangle_0$ is the expected value of B with respect to f_0 . Thanks to the relation (4.31), the linear response (4.30), F function (4.25) and G function (4.26) are rewritten in the forms of

$$\langle \tilde{B} \rangle_1(\omega) = -\langle \{\tilde{B}_{\omega}, v \cdot (I - \tilde{F}(\omega))^{-1} \tilde{G}(\omega) + \tilde{H}_1(\omega)\} \rangle_0, \quad (4.32)$$

$$\tilde{F}_{kl}(\omega) = -V_l \langle \{\tilde{E}_{\omega}^k, E^{-l}\} \rangle_0, \quad (4.33)$$

and

$$\tilde{G}_k(\omega) = -\frac{1}{2\pi} \langle \{\tilde{E}_\omega^k, \tilde{H}_1(\omega)\} \rangle_0, \quad (4.34)$$

respectively.

4.3 \tilde{F} and \tilde{G} functions

The linear response (4.30) is determined by F and G functions. We therefore explicitly compute F and G functions both for spatially homogeneous and inhomogeneous stationary state f_0 . We assume that f_0 depends on (q, p) only through $\mathcal{H}_0[f_0]$, and then $f_0(q, p) = \tilde{f}_0(\mathcal{H}_0[f_0](q, p))$ is a stationary solution satisfying Eq. (4.7).

4.3.1 Homogeneous case

Let us consider the case that the stationary state f_0 is spatially homogeneous. Omitting the constant of potential, which is irrelevant to dynamics, the single-body Hamiltonian $\mathcal{H}_0[f_0]$ is written as

$$\mathcal{H}_0[f_0] = \frac{p^2}{2}. \quad (4.35)$$

The Hamiltonian flow ϕ_0^t is hence expressed by the simple form of

$$\phi_0^t(q, p) = (q + tp, p). \quad (4.36)$$

The function $E_t^k(q, p)$ is therefore

$$E_t^k(q, p) = e^{-ik(q+tp)}, \quad (4.37)$$

and its Laplace transform is

$$\tilde{E}_\omega^k(q, p) = \frac{-e^{-ikq}}{i(\omega - kp)}. \quad (4.38)$$

Performing the Fourier series expansion of H_1 with respect to q , the F function and the G function are expressed by

$$\tilde{F}_{kl}(\omega) = -2\pi k V_k \delta_{k,l} \int_L \frac{f_0'(p)}{\omega - kp} dp \quad (4.39)$$

and

$$\tilde{G}_k(\omega) = -k \int_L \frac{f_0'(p)}{\omega - kp} \tilde{H}_{1,k}(p, \omega) dp. \quad (4.40)$$

The functions (4.39) and (4.40) vanish for $k = 0$ and we may set $k \neq 0$. The functions are defined in the upper half ω plane due to the Laplace transform (4.23), and we must consider analytic continuation for extending the domain to the whole ω plane. The integral path L is the real p axis for $\text{Im}\omega > 0$, but is continuously modified to avoid the singularity at $p = \omega/k$ for $\text{Im}\omega \leq 0$ as $\text{Im}\omega$ goes down. The functions hence pick up contribution from the pole for $\text{Im}\omega \leq 0$ in addition to the integral on the real p axis [Lan1946, LP1981].

The matrix F is diagonal, and Eq. (4.27) can be solved in each element as

$$\tilde{\rho}_{1,k}(\omega) = \frac{\tilde{G}_k(\omega)}{D_k(\omega)}, \quad (4.41)$$

where

$$D_k(\omega) = 1 + 2\pi k V_k \int_L \frac{f'_0(p)}{\omega - kp} dp \quad (4.42)$$

is the dielectric function or the dispersion function. Moreover, if H_1 does not depend on p , then we can write the density $\tilde{\rho}_{1,k}$ by

$$\tilde{\rho}_{1,k}(\omega) = \frac{\tilde{H}_{1,k}(\omega)}{2\pi V_k} \frac{1 - D_k(\omega)}{D_k(\omega)} \quad (4.43)$$

for modes of $V_k \neq 0$. We note that V_k is defined in Eq. (4.17), and it is not a Fourier coefficient of $\mathcal{V}[f_0]$ but of $V(q)$. There must be some nonzero coefficients V_k for $k \neq 0$ even for spatially homogeneous f_0 , since the Hamiltonian system (4.1) is supposed to have long-range interaction.

We exhibit trivial but important examples of the linear response. We assume that Eq. (4.31) holds. Choosing the observable $B(q, p)$ in Eq. (4.14) as a function $g(p)$ depending on p only, g_t is identical with g by Eq. (4.36). The linear response of g is hence

$$\langle g \rangle_1 = \int_0^t ds \iint_{\mu} \{g_{t-s}, f_0\} [\mathcal{V}[f_1](s) + H_1(s)] dq dp = 0, \quad (4.44)$$

since $\{g_{t-s}, f_0\} = 0$. Setting $g(p) = p^2$, we obtain that the kinetic temperature $T_{\text{kin}} = \langle p^2 \rangle$ is not affected by the external field within accuracy of order $O(H_1)$. We further remark that the vanishing expectation value (4.44) holds in systems with periodic boundary condition, but may break in a system, for instance, gas confined by walls, since the relation (4.31) is not guaranteed to hold.

4.3.2 Inhomogeneous case

Suppose that the stationary state f_0 is spatially inhomogeneous. To get the Hamiltonian flow ϕ_0^t , we transform the Cartesian coordinate (q, p) to the angle-action variables (θ, J) . This transform is not always injective on the whole μ space, and must be defined on each of divided spaces to make the transform bijective. See Section 2.4.2 for the HMF case.

The single-body Hamiltonian is integrable, and is a function of J only as $\mathcal{H}_0[f_0](J)$. Defining frequency

$$\Omega(J) = \frac{d\mathcal{H}_0[f]}{dJ}(J), \quad (4.45)$$

the Hamiltonian flow ϕ_0^t is written as

$$\phi_0^t(\theta, J) = (\theta + t\Omega(J), J). \quad (4.46)$$

Let us compute \tilde{E}_ω^k , which appears in F and G functions, by using the angle-action variables.

The function E^k is periodic with respect to θ , and hence it is expanded in the Fourier series as

$$E^k(\theta, J) = e^{-ikq(\theta, J)} = \sum_{m \in \mathbb{Z}} E^{k,m}(J) e^{im\theta}, \quad (4.47)$$

where

$$E^{k,m}(J) = \frac{1}{2\pi} \int_{-\pi}^{\pi} e^{-ikq(\theta, J)} e^{-im\theta} d\theta. \quad (4.48)$$

Using Eq. (4.46), the function E_t^k is expressed by

$$E_t^k(\theta, J) = \sum_{m \in \mathbb{Z}} E^{k,m}(J) e^{im(\theta + t\Omega(J))}, \quad (4.49)$$

and the function \tilde{E}_ω^k is

$$\tilde{E}_\omega^k(\theta, J) = \sum_{m \in \mathbb{Z}} E^{k,m}(J) e^{im\theta} \frac{-1}{i(\omega + m\Omega(J))}. \quad (4.50)$$

The transform $(q, p) \mapsto (\theta, J)$ is canonical, and hence the Poisson bracket is invariant under this transform, and $dq \wedge dp = d\theta \wedge dJ$ holds. The F and G functions are thus

$$\tilde{F}_{kl}(\omega) = -2\pi V_l \sum_{m \in \mathbb{Z}} m \int_L \frac{f'_0(J)}{\omega - m\Omega(J)} E^{k,-m}(J) E^{-l,m}(J) dJ, \quad (4.51)$$

and

$$\tilde{G}_k(\omega) = - \sum_{m \in \mathbb{Z}} m \int_L \frac{f'_0(J)}{\omega - m\Omega(J)} E^{k,-m}(J) \tilde{H}_{1,m}(J, \omega) dJ, \quad (4.52)$$

respectively. The functions (4.51) and (4.52) are defined in the upper half ω plane, and the integral path L lies on the real axis. As done in the homogeneous case, the path L is modified to obtain analytic continuation to the whole ω plane.

We note that the vanishing expectation value (4.44) is not always guaranteed for spatially inhomogeneous stationary state even if we set g as a function of J only. The domain of J is, for instance, $[0, \infty)$, and contribution from $J = 0$ may remain in the relation (4.31) in the way of integration by parts.

4.4 Linear response theory in Hamiltonian mean-field model

We apply the linear response theory to the Hamiltonian mean-field (HMF) model. We summarize the theory for HMF model in this section, and examine the theory in the following two sections, Sections 4.3.1 and 4.3.2, for homogeneous and for inhomogeneous cases respectively.

The HMF model is a ferromagnetic model, and is expressed by taking

$$V(q) = -\cos q. \quad (4.53)$$

We introduce magnetization (M_x, M_y) as

$$\begin{aligned} M_x[f](t) &= \iint_{\mu} f(q, p, t) \cos q \, dq dp, \\ M_y[f](t) &= \iint_{\mu} f(q, p, t) \sin q \, dq dp, \end{aligned} \quad (4.54)$$

and denote the response parts by $M_{1,x}(t) = M_x[f_1](t)$ and $M_{1,y}(t) = M_y[f_1](t)$. The single-body Hamiltonian for the HMF model is

$$\mathcal{H}_0[f](q, p, t) = \frac{p^2}{2} - M_x[f](t) \cos q - M_y[f](t) \sin q, \quad (4.55)$$

and the external field H_1 can be set by

$$H_1(q, p, t) = -h_x(t) \cos q - h_y(t) \sin q, \quad (4.56)$$

where h_x and h_y are time-dependent external magnetic fields for x -direction and y -direction respectively.

Using $\cos q$ and $\sin q$ instead of e^{iq} and e^{-iq} , and writing them by

$$C(q, p) = \cos q, \quad S(q, p) = \sin q, \quad (4.57)$$

we obtain

$$\begin{pmatrix} \tilde{M}_{1,x}(\omega) \\ \tilde{M}_{1,y}(\omega) \end{pmatrix} = \begin{pmatrix} \tilde{F}_{cc}(\omega) & \tilde{F}_{cs}(\omega) \\ \tilde{F}_{sc}(\omega) & \tilde{F}_{ss}(\omega) \end{pmatrix} \begin{pmatrix} \tilde{M}_{1,x}(\omega) \\ \tilde{M}_{1,y}(\omega) \end{pmatrix} + \begin{pmatrix} \tilde{G}_c(\omega) \\ \tilde{G}_s(\omega) \end{pmatrix}, \quad (4.58)$$

where

$$\begin{aligned} \tilde{F}_{cc}(\omega) &= \iint_{\mu} \tilde{C}_{\omega}\{C, f_0\} \, dq dp, & \tilde{F}_{cs}(\omega) &= \iint_{\mu} \tilde{C}_{\omega}\{S, f_0\} \, dq dp, \\ \tilde{F}_{sc}(\omega) &= \iint_{\mu} \tilde{S}_{\omega}\{C, f_0\} \, dq dp, & \tilde{F}_{ss}(\omega) &= \iint_{\mu} \tilde{S}_{\omega}\{S, f_0\} \, dq dp, \end{aligned} \quad (4.59)$$

and

$$\begin{aligned} \tilde{G}_c(\omega) &= - \iint_{\mu} \tilde{C}_{\omega}\{\tilde{H}_1(\omega), f_0\} \, dq dp, \\ \tilde{G}_s(\omega) &= - \iint_{\mu} \tilde{S}_{\omega}\{\tilde{H}_1(\omega), f_0\} \, dq dp. \end{aligned} \quad (4.60)$$

The external field (4.56) gives

$$\begin{pmatrix} \tilde{G}_c(\omega) \\ \tilde{G}_s(\omega) \end{pmatrix} = \begin{pmatrix} \tilde{F}_{cc}(\omega) & \tilde{F}_{cs}(\omega) \\ \tilde{F}_{sc}(\omega) & \tilde{F}_{ss}(\omega) \end{pmatrix} \begin{pmatrix} \tilde{h}_x(\omega) \\ \tilde{h}_y(\omega) \end{pmatrix}, \quad (4.61)$$

and hence Eq. (4.58) is solved as

$$\begin{pmatrix} \tilde{M}_{1,x}(\omega) \\ \tilde{M}_{1,y}(\omega) \end{pmatrix} = \left(I - \tilde{F}(\omega) \right)^{-1} \tilde{F}(\omega) \begin{pmatrix} \tilde{h}_x(\omega) \\ \tilde{h}_y(\omega) \end{pmatrix}. \quad (4.62)$$

The off diagonal elements of the matrix F vanish as

$$\tilde{F}_{cs}(\omega) = \tilde{F}_{sc}(\omega) = 0 \quad (4.63)$$

in the homogeneous case. The relation (4.63) is also satisfied in the inhomogeneous case [BOY2010]. The response of magnetization is therefore written as

$$\begin{aligned} \tilde{M}_{1,x}(\omega) &= \frac{1 - D_x(\omega)}{D_x(\omega)} \tilde{h}_x(\omega), \\ \tilde{M}_{1,y}(\omega) &= \frac{1 - D_y(\omega)}{D_y(\omega)} \tilde{h}_y(\omega), \end{aligned} \quad (4.64)$$

where

$$D_x(\omega) = 1 - \tilde{F}_{cc}(\omega), \quad D_y(\omega) = 1 - \tilde{F}_{ss}(\omega) \quad (4.65)$$

are the dispersion functions for x -direction and y -direction, respectively. The concrete forms of $F_{cc}(\omega)$ and $F_{ss}(\omega)$ are expressed by

$$\tilde{F}_{cc}(\omega) = \tilde{F}_{ss}(\omega) = -\pi \int_L \frac{f'_0(p)}{p - \omega} dp \quad (4.66)$$

for the homogeneous case and

$$\begin{aligned} \tilde{F}_{cc}(\omega) &= -2\pi \sum_m \int_L \frac{mf'_0(J)}{m\Omega(J) - \omega} |C^m(J)|^2 dJ, \\ \tilde{F}_{ss}(\omega) &= -2\pi \sum_m \int_L \frac{mf'_0(J)}{m\Omega(J) - \omega} |S^m(J)|^2 dJ, \end{aligned} \quad (4.67)$$

for the inhomogeneous case. Here we introduced new functions

$$\begin{aligned} C^m(J) &= \frac{1}{2\pi} \int \cos q(\theta, J) e^{-im\theta} d\theta, \\ S^m(J) &= \frac{1}{2\pi} \int \sin q(\theta, J) e^{-im\theta} d\theta. \end{aligned} \quad (4.68)$$

We note that the expression (4.64) is valid both for homogeneous and for inhomogeneous cases by selecting F_{cc} as Eq. (4.66) for the homogeneous case and as Eq. (4.67) for the inhomogeneous case.

Let us consider the asymptotic behavior of $M_{1,x}$ and $M_{1,y}$. There is no difference between $M_{1,x}$ and $M_{1,y}$ in Eq. (4.64) formally, and hence we focus on $M_{1,x}$ by setting

$$h_x(t) = h\Theta(t) \cos \omega_0 t, \quad (4.69)$$

where $\Theta(t)$ is the step function. The Laplace transform of $h_x(t)$ is

$$\tilde{h}_x(\omega) = \frac{-h}{2i} \left(\frac{1}{\omega - \omega_0} + \frac{1}{\omega + \omega_0} \right) \quad (4.70)$$

and hence temporal evolution $M_{1,x}(t)$ is

$$M_{1,x}(t) = \frac{-h}{4\pi i} \int_{\Gamma} \frac{1 - D_x(\omega)}{D_x(\omega)} \left(\frac{1}{\omega - \omega_0} + \frac{1}{\omega + \omega_0} \right) e^{-i\omega t} d\omega, \quad (4.71)$$

where Γ is a Bromwich contour running from $-\infty + i\sigma$ to $+\infty + i\sigma$ with a real positive σ , which is set such that all singularities of the integrand are below of this Bromwich contour. In the inhomogeneous case $D_x(\omega)$ has logarithmic singularities and branch points are on the real axis [BOY2010, BOY2011]. However, we neglect the logarithmic singularities and concentrate on pole singularities. In other words we assume that ω_0 is not at the branch points. We will discuss on the logarithmic singularities in Section 4.8.

Suppose that all roots of $D_x(\omega)$ are on the lower-half ω plane, and they give exponential Landau dampings [Lan1946, LP1981]. Asymptotic behavior of $M_{1,x}(t)$ is then determined by the poles at $\omega = \pm\omega_0$, and

$$M_{1,x}(t) \rightarrow \frac{h}{2} \left(\frac{1 - D_x(\omega_0)}{D_x(\omega_0)} e^{-i\omega_0 t} + \frac{1 - D_x(-\omega_0)}{D_x(-\omega_0)} e^{i\omega_0 t} \right). \quad (4.72)$$

In particular, setting $\omega_0 = 0$, we have

$$M_{1,x}(t) \rightarrow h \frac{1 - D_x(0)}{D_x(0)}. \quad (4.73)$$

For the external field of y-direction,

$$h_y(t) = h\Theta(t) \cos \omega_0 t, \quad (4.74)$$

we obtain the same results for $M_{1,y}(t)$ by replacing x with y in Eqs. (4.72) and (4.73).

We remark on asymptotic values of $M_{1,x}(t)$ and $M_{1,y}(t)$ for $\omega_0 = 0$. Let us focus on $M_{1,x}(t)$ without loss of generality. We used the step function $\Theta(t)$ in $h_x(t)$, and the Laplace transform of $h_x(t)$ is therefore expressed by

$$\tilde{h}_x(\omega) = \frac{-h}{i\omega} \quad (4.75)$$

for $\omega_0 = 0$. This singularity at the origin $\omega = 0$ leads the asymptotic form (4.73) by the inverse Laplace transform. However, the step function is not essential to give the singularity at the origin $\omega = 0$, and any smooth functions give the same singularity if the functions go to a constant in the limit $t \rightarrow \infty$. See Appendix C.2 for details.

4.5 Response in homogeneous case

We add a non-oscillating external field, say, $\omega_0 = 0$, and use Eq. (4.73) to investigate Curie-Weiss law like behavior of the susceptibility in the homogeneous case. We may set that the external field points to x -direction without loss of generality thanks to rotational symmetry in the homogeneous case. The external field is hence set as $(h_x(t), h_y(t)) = (h\Theta(t), 0)$. We will use energy U to identify

the critical point, where energy in the HMF model is defined by

$$U = \iint \frac{p^2}{2} f dq dp + \frac{1}{2} - \frac{M_x^2 + M_y^2}{2}. \quad (4.76)$$

The constant $1/2$ in the right-hand side is added for convenience of comparison with previous studies of the HMF model.

4.5.1 Thermal equilibrium

The first example is thermal equilibrium,

$$f_0(p) = \frac{1}{2\pi} \sqrt{\frac{\beta}{2\pi}} e^{-\beta p^2/2}. \quad (4.77)$$

The critical energy of a second-order phase transition is $U_c = 3/4$, which corresponds to the critical temperature $T_c = 1/2$. We chose the unit so the Boltzmann's constant is unity, $k_B = 1$.

The dispersion function at $\omega = 0$ is

$$D_1(0) = 1 - \frac{\beta}{2} \quad (4.78)$$

and the asymptotic linear response of $M_{1,x}$ is

$$M_{1,x} = h \frac{\beta/2}{1 - \beta/2} = h \frac{T_c}{T - T_c}. \quad (4.79)$$

The susceptibility χ , defined by

$$\chi = \lim_{h \rightarrow 0} \frac{M_{1,x}}{h} = \frac{T_c}{T - T_c}, \quad (4.80)$$

and χ diverges at the critical point. This susceptibility is rewritten

$$\chi = \frac{1}{3} \frac{U_c}{U - U_c}, \quad (4.81)$$

where we used the relation $T = 2U - 1$ in the high-energy, homogeneous region, $U > U_c = 3/4$. We note that this form (4.81) of susceptibility can be also obtained by computing the N -body partition function and by using the minimum free energy principle for a functional of the single-body distribution function [Cha2011a].

4.5.2 Power-law tails

The second example is a family of distributions having power-law tails as

$$f_\nu(p) = \frac{1}{2\pi} \frac{A_\nu(p_0)}{1 + |p/p_0|^\nu}. \quad (4.82)$$

Exactly saying, this family is not smooth at $p = 0$ except for even ν and, hence, is not suitable to consider analytic continuation to obtain the dispersion function $D_x(0)$. However, we apply the linear response theory to this family formally.

The parameter p_0 is determined by the kinetic energy $K = \iint_{\mu} (p^2/2) f_{\nu}(p) dq dp$ as

$$p_0 = \sqrt{2K(3 - 4 \sin^2(\pi/\nu))} \quad (4.83)$$

and the normalization factor $A_{\nu}(p_0)$ is expressed by

$$A_{\nu}(p_0) = \frac{\nu}{2\pi p_0} \sin\left(\frac{\pi}{\nu}\right) \quad (4.84)$$

for $\nu > 2$ [YBD2007]. This family gives a second-order phase transition at the critical energy

$$U_c^{\nu} = \frac{1}{2} + \frac{1}{4(3 - 4 \sin^2(\pi/\nu))} \quad (4.85)$$

for $\nu > 3$. The dispersion function is computed as

$$D_{\nu}(0) = 1 + \pi \int_{-\infty}^{\infty} \frac{f'_{\nu}(p)}{p} dp = 1 - \frac{1}{2p_0^2}, \quad (4.86)$$

and hence the susceptibility is

$$\chi_{\nu} = C_{\nu} \frac{U_c^{\nu}}{U - U_c^{\nu}}, \quad (4.87)$$

where the factor C_{ν} is

$$C_{\nu} = \frac{1}{7 - 8 \sin^2(\pi/\nu)} \quad (4.88)$$

We remark that the critical energy (4.85) and the constant (4.88) coincide with ones for thermal equilibrium by taking $\nu = 4$, which gives $(U_c^4, C_4) = (3/4, 1/3)$. Taking the limit of $\nu \rightarrow \infty$, the distribution (4.82) becomes a homogeneous waterbag, and gives $(U_c^{\nu}, C_{\nu}) \rightarrow (7/12, 1/7)$. We also remark that C_{ν} is an decreasing function of ν and ν must be $\nu > 3$ to converge energy U . The range of C_{ν} is thus $1/7 < C_{\nu} < 1$. In particular, in the interval $3 < \nu < 4$, where the critical energy U_c^{ν} is larger than $3/4$, C_{ν} is larger than the value $1/3$ for thermal equilibrium.

4.5.3 Lynden-Bell distribution

The third example is a family of Lynden-Bell distributions

$$f_{\text{LB}}(p) = \frac{f_1}{e^{\alpha + \beta p^2/2} + 1}. \quad (4.89)$$

This family is expected as a quasi-stationary state starting from a rectangle waterbag initial state [AFB+2007, AFRY2007], and we parametrize this family by energy U and the magnetization

M_{wb} of the waterbag state. Distribution of the waterbag is written in the form

$$f_{\text{wb}}(q, p) = \begin{cases} f_1 & (|q| < \Delta q \text{ and } |p| < \Delta p), \\ 0 & (\text{otherwise}). \end{cases} \quad (4.90)$$

The two parameters Δq and Δp determine the factors f_1 , the magnetization M_{wb} and energy U as

$$f_1 = \frac{1}{4\Delta q\Delta p}, \quad M_{\text{wb}} = \frac{\sin \Delta q}{\Delta q}, \quad U = \frac{\Delta p^2}{6} + \frac{1 - M_{\text{wb}}^2}{2}. \quad (4.91)$$

The Lagrange multipliers α and β included in Eq. (4.89) are determined by the two constraints

$$\iint_{\mu} f_{\text{LB}}(p) dq dp = 1 \quad (4.92)$$

and

$$\iint_{\mu} \frac{p^2}{2} f_{\text{LB}}(p) dq dp + \frac{1}{2} = U. \quad (4.93)$$

We stress that the parameters M_{wb} and U are used just to parametrize the family (4.89) for convenience of comparison with previous works, and the stationary state f_0 is set as f_{LB} instead of f_{wb} . In other words, we do not consider the violent relaxation process from the waterbag to the Lynden-Bell distribution.

The family (4.89) has a tricritical point at $(M_{\text{wb}}^{\text{tc}}, U_{\text{tc}})$ on the parameter plane (M_{wb}, U) [OY2011], and there is a second-order phase transition along an iso- M_{wb} line for $M_{\text{wb}} > M_{\text{wb}}^{\text{tc}}$, and a first-order phase transition for $M_{\text{wb}} < M_{\text{wb}}^{\text{tc}}$. Even for $M_{\text{wb}} < M_{\text{wb}}^{\text{tc}}$, a spatially homogeneous Lynden-Bell distribution is locally stable in a high-energy region. The stable region is expressed by the inequality

$$D_x(0) > 0, \quad (4.94)$$

and $D_x(0) = 0$ gives the critical energy $U_c(M_{\text{wb}})$ as shown in Fig. 4.1. Using this critical energy, the susceptibility χ is expressed by

$$\chi = \frac{1 - D_x(0)}{D_x(0)} = C(M_{\text{wb}})u^{-\gamma(M_{\text{wb}})}, \quad u = \frac{U - U_c}{U_c}. \quad (4.95)$$

We check if the Curie-Weiss like law, $\gamma(M_{\text{wb}}) = 1$, is satisfied even in QSSs by computing $D_x(0)$ and by direct temporal evolutions of the Vlasov equation.

The Vlasov equation is evolved by use of the semi-Lagrangian method [deB2010]. We denote the number of grid points for q and p directions by N_q and N_p respectively. The time slice is fixed as $\Delta t = 0.05$. We introduce cut-off for the p direction and the computed interval of p is $[-20, 20]$. Strength of the external field is $h = 0.005$.

The normalized response M_x/h , where $M_x = M_{1,x}$ in the homogeneous case, is shown in Fig. 4.2 as a function of $u = (U - U_c)/U_c$ along the iso- M_{wb} line with $M_{\text{wb}} = 0.5$. The theoretical line seems almost straight, while semi-Lagrangian method gives non-straight curve for small u , namely $u < 0.1$. This is because the size of the external field $h = 0.005$ is too large.

In order to compute the exponent $\gamma(M_{\text{wb}})$ and the factor $C(M_{\text{wb}})$, we apply the least mean square method for various intervals of u . Computed $\gamma(M_{\text{wb}})$ and $C(M_{\text{wb}})$ are exhibited in Fig.

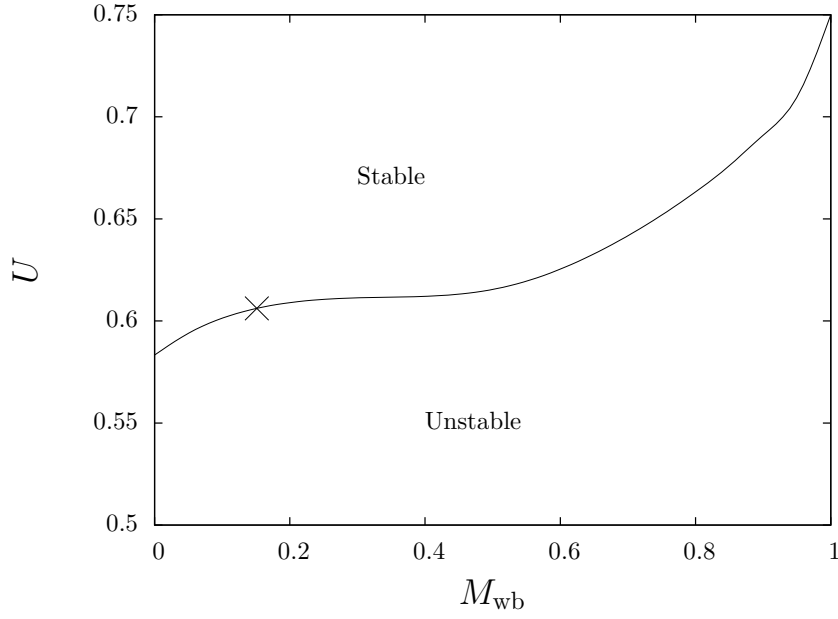


Figure 4.1: Critical line determined by $D_x(0) = 0$. The cross point represents the tricritical point [OY2011]. Spatially homogeneous state is stable or metastable in the upper side of the critical line, and is unstable in the lower side.

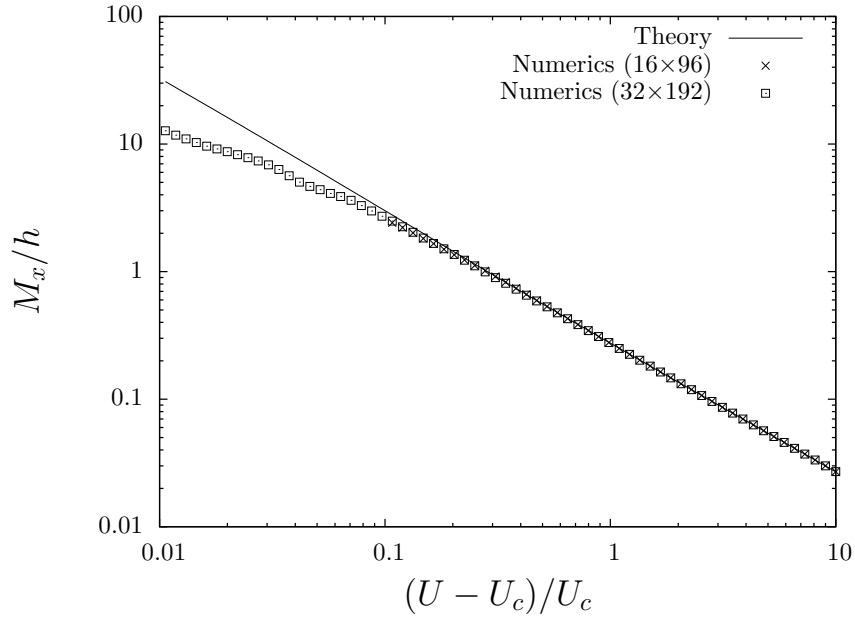


Figure 4.2: Normalized response M_x/h as a function of normalized energy $u = (U - U_c)/U_c$ along iso- M_{wb} line with $M_{wb} = 0.5$. $h = 0.005$. The line is obtained by use of the theory, and the points are obtained by use of the semi-Lagrangian method. Crosses are for $N_q = 16$ and $N_p = 96$, and squares for $N_q = 32$ and $N_p = 192$. The points are averages of $M_x(t)$ in the time interval $t \in [200, 500]$.

4.3. The theoretical exponent $\gamma(M_{\text{wb}})$ is not the unity, but damps to the unity as the interval excludes low-energy region. We remark that, for the interval $u \in [1, 10]$, $\gamma(M_{\text{wb}})$ and $C(M_{\text{wb}})$ for $N_q = 16$ and $N_p = 96$ coincide with ones for $N_q = 32$ and $N_p = 192$ respectively, though the result for the former is not reported. We therefore may conclude that a Curie-Weiss like law, $M_x/h \propto 1/u$, appears in an asymptotic high-energy region.

The factor $C(M_{\text{wb}})$ monotonically increases as M_{wb} increases, and is not almost affected by choice of the interval of u . In particular, in a high-energy region $u \in [1, 10]$, the semi-Lagrangian method is in good agreement with the theory. The susceptibility is hence written in the Curie-Weiss like law $\chi = C(M_{\text{wb}})/u$ in the high-energy region.

We also computed the exponent $\gamma(M_{\text{wb}})$ and the factor $C(M_{\text{wb}})$ from equations derived by the Sommerfeld expansion reported in Ref. [PGN2012]. The Sommerfeld expansion breaks around $M_{\text{wb}} \simeq 0.2$ since a large M_{wb} gives a small β in Eq. (4.89), while the expansion assumes a large β .

4.5.4 Momentum deviation and C factor

We considered three types of distributions, thermal equilibrium, power-law tails and Lynden-Bell distributions, and the Curie-Weiss like law is satisfied, at least in the high-energy region. Factor C depends on a considering family of stationary distributions, and it tends to increase as momentum deviation becomes large. Is there universality in the relation between the factor C and momentum deviation?

The factor C is reported in Fig. 4.4 as a function of momentum deviation σ_p^2 at the critical point. It is true that C is an increasing function of σ_p^2 , but no universality is found. This non-universality suggests possibility that a type of distribution family of QSSs could be detected by computing factor C if the family has a second-order phase transition. However, we need further investigations of critical phenomena in QSSs to perform this detection.

4.6 Response in inhomogeneous case

We now investigate the linear response in the inhomogeneous case. We use thermal equilibrium as a family of QSSs, which are expressed by

$$f_0(q, p) = A e^{-\beta(p^2/2 - M_0 \cos q)}, \quad (4.96)$$

where A is the normalization factor. The 0-th order magnetization M_0 points to the x -direction and must satisfy the self-consistent equation

$$M_0 = \iint f_0(q, p) \cos q \, dq dp. \quad (4.97)$$

We consider the linear response to non-oscillating external fields in Section 4.6.1, and resonance absorption by oscillating fields in Section 4.6.2.

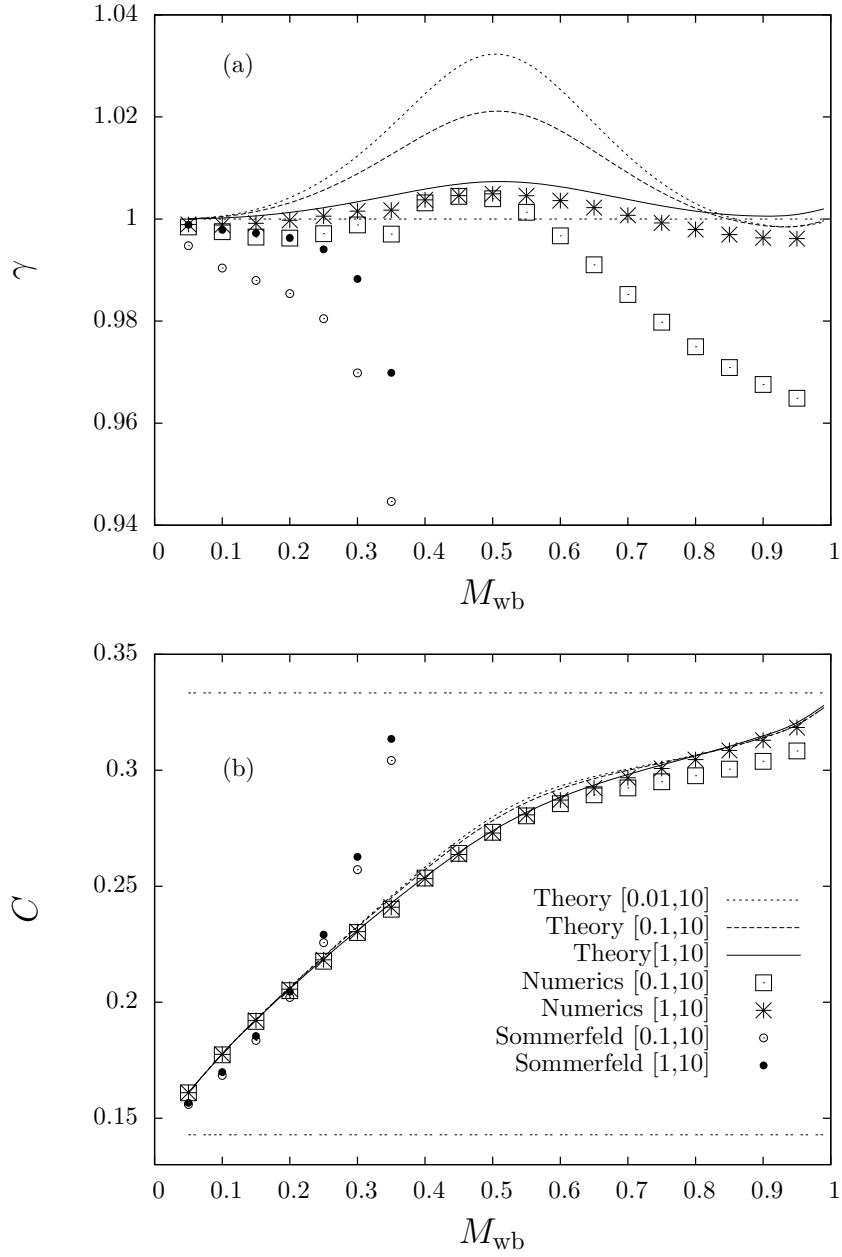


Figure 4.3: M_{wb} dependence of (a) exponent $\gamma(M_{wb})$ and (b) factor $C(M_{wb})$, which are defined by Eq. (4.95). Lines are obtained by the theory, big points by the semi-Lagrangian method, and small circle points by Sommerfeld expansion reported in Ref. [PGN2012]. Dashed line is computed by use of the least mean square method applied to the interval $u \in [0.01, 10]$. Broken line, square points and white small points are for $u \in [0.1, 10]$. Star points and black small points are for $u \in [1, 10]$. Two horizontal lines in the panel (b) represent $1/3$ (upper) and $1/7$ (lower), which are theoretically obtained factors for thermal equilibrium and waterbag respectively.

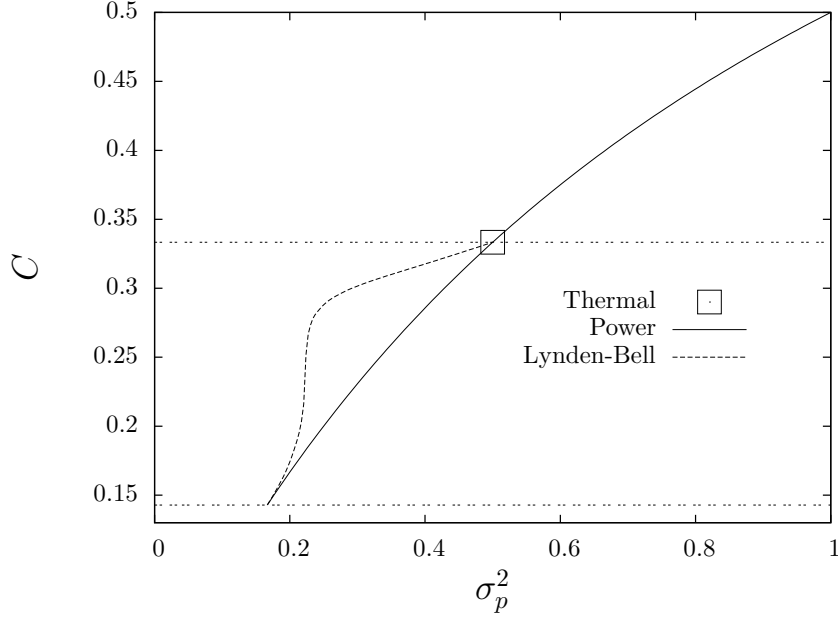


Figure 4.4: Factor C as a function of momentum deviation at the critical point. Square point is for thermal equilibrium, solid line is for power tails and broken line is for Lynden-Bell.

4.6.1 Response to non-oscillating external field

In the inhomogeneous case, the rotational symmetry breaks and we separately consider two types of external fields which point to x -direction and to y -direction.

An external field to the x -direction is expressed by $(h_x(t), h_y(t)) = (h\Theta(t), 0)$. The response $M_{1,x}$ is expressed by Eq. (4.73), and the concrete form of the dispersion function at $\omega = 0$, $D_x(0)$, is written by using elliptic integrals as follows.

Let us introduce a variable

$$k = \sqrt{\frac{M_0 + \mathcal{E}}{2M_0}} \quad (4.98)$$

with the single body energy

$$\mathcal{E} = \frac{p^2}{2} - M_0 \cos q. \quad (4.99)$$

As we assumed before, the stationary state $f_0(q, p)$ depends on q and p through the single-body energy and hence through k only, that is,

$$f_0(q, p) = \bar{f}_0(k). \quad (4.100)$$

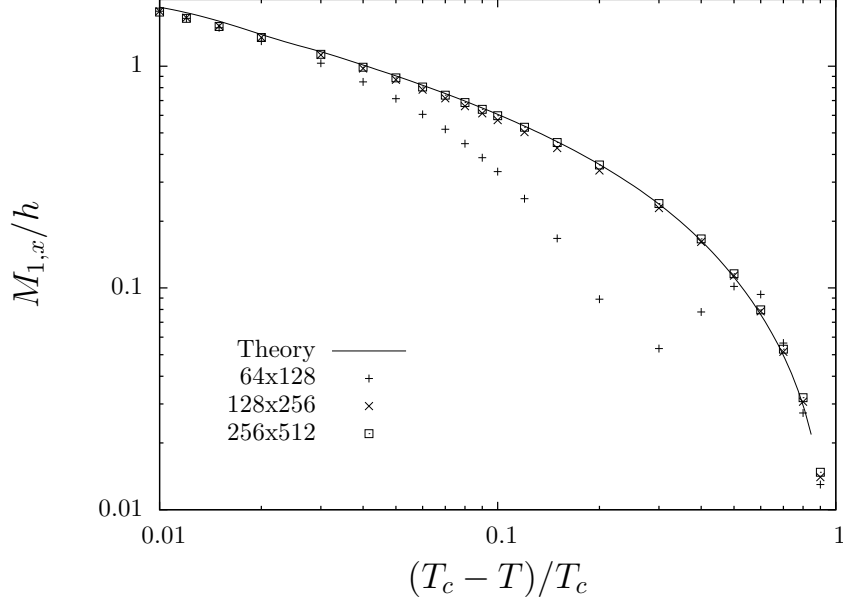


Figure 4.5: Response $M_{1,x}/h$ as a function of $(T_c - T)/T_c$ with $T_c = 1/2$. $h = 0.005$. The line is obtained by the theory, and the points by the semi-Lagrangian method. The value of $M_{1,x}$ in the semi-Lagrangian method is averaged over the time interval $t \in [200, 500]$. The numbers in panel represent the size of grid $N_q \times N_p$.

Using \bar{f}_0 , the dispersion function $D_x(0)$ is written in the form

$$\begin{aligned}
D_x(0) = 1 &+ \iint_{\mu} \frac{1}{p} \frac{\partial f_0}{\partial p}(q, p) \cos^2 q \, dq dp \\
&- \frac{4}{\sqrt{M_0}} \int_1^{\infty} \frac{K(1/k)}{k} \left(\frac{2k^2 E(1/k)}{K(1/k)} + 1 - 2k^2 \right)^2 \frac{d\bar{f}_0}{dk}(k) \, dk \\
&- \frac{4}{\sqrt{M_0}} \int_0^1 K(k) \left(\frac{2E(k)}{K(k)} - 1 \right)^2 \frac{d\bar{f}_0}{dk}(k) \, dk,
\end{aligned} \tag{4.101}$$

where $K(k)$ and $E(k)$ are the complete elliptic integrals of the first and the second kinds respectively. We have derived it in Section 3.4.1. The theoretical linear response is obtained by computing $D_x(0)$ and substituting it into Eq. (4.73). The theoretical prediction is reported in Fig. 4.5 with numerical results of the semi-Lagrangian method. The theoretical curve is in good agreement with numerics of the grid sizes $N_q \times N_p = 128 \times 256$ and 256×512 .

We also consider response to the external field to the y-direction, $(h_x(t), h_y(t)) = (0, h\Theta(t))$. The concrete form of $D_y(0)$ is

$$D_y(0) = 1 + \iint_{\mu} \frac{1}{p} \frac{\partial f_0}{\partial p}(q, p) \sin^2 q \, dq dp, \tag{4.102}$$

and $D_y(0) = 0$ as shown in Section 3.4.1. The susceptibility for the y-direction therefore diverges. This divergence is consistent with the fact that the magnetization vector (M_x, M_y) can turn, holding its modulus, to arbitrary direction with arbitrary small work.

4.6.2 Resonance absorption and exploring Landau pole

We apply the linear response theory for extracting non-equilibrium dynamics in the unforced system through resonance absorption for oscillating external fields. The HMF system has “Landau dampings” even in the inhomogeneous case, and there are several Landau poles corresponding to roots of the dispersion function, $\det(I - \tilde{F}(\omega))$. The imaginary part of the roots is negative if the stationary state f_0 is stable. The most important root is the one whose imaginary part is the largest, since the damping rate corresponding to the root is the smallest. We call this root the main root and denote $\omega_L = \omega_1 + i\omega_2$, $\omega_1, \omega_2 \in \mathbb{R}$. Detecting the main root has been explicitly done for inhomogeneous thermal equilibrium of the HMF model [BOY2010], but this detection is a hard task since logarithmic singularities appear in F and G functions. We therefore try to capture “Landau dampings” in inhomogeneous states from the view point of resonance absorption.

Let us consider the external field vector pointing to x -direction, that is, $(h_x(t), 0)$ and $h_x(t)$ is represented by Eq. (4.69). In a short time interval, the external field $h_x(t)$ induces a small modification of magnetization denoted by $dM_{1,x}(t)$. The work by the external field is, hence, expressed by

$$dW = h_x(t)dM_{1,x}(t), \quad (4.103)$$

and the average over one period is computed as

$$\begin{aligned} \overline{W} &= \frac{\omega_0}{2\pi} \int_0^{2\pi/\omega_0} h_x(t) \frac{dM_x}{dt}(t) dt \\ &= \frac{-ih^2\omega_0}{4} \left(\frac{1 - D_x(\omega_0)}{D_x(\omega_0)} - \frac{1 - D_x(-\omega_0)}{D_x(-\omega_0)} \right), \end{aligned} \quad (4.104)$$

where we used asymptotic expression of $M_{1,x}(t)$ [Eq. (4.72)].

The dispersion function $D_x(\omega)$ satisfies the relation

$$D_x(-\omega^*) = D_x(\omega)^*, \quad (4.105)$$

where ω^* is the complex conjugate of ω . The work is, for a real ω_0 , therefore expressed by

$$\overline{W} = \frac{h^2\omega_0}{2} \text{Im} \left(\frac{1 - D_x(\omega_0)}{D_x(\omega_0)} \right). \quad (4.106)$$

Moreover, if ω_L is a main root, then $-\omega_L^* = -\omega_1 + i\omega_2$ is also a main root. We can hence write $D_x(\omega)$ in the form

$$D_x(\omega) = (\omega - \omega_L)(\omega + \omega_L^*)\varphi(\omega). \quad (4.107)$$

To estimate the maximum work as a function of ω_0 , we introduce two assumptions. (i) $1 - D_x(\omega_0) \simeq 1$. (ii) $\varphi(\omega_0)$ is a constant φ_0 . These assumptions lead the fact that φ_0 is a real number, and consequently \overline{W} takes the maximum value

$$\overline{W}_{\max} = \frac{h^2}{4\omega_2\varphi_0} \quad (4.108)$$

at frequency

$$\omega_0 = \pm|\omega_L|. \quad (4.109)$$

Table 4.1: Comparison between $|\omega_L|$ and peak positions of Fig. 4.6. Real and imaginary parts of ω_L are read from Figs.11 and 10 of Ref. [BOY2010] respectively. In the line of “Peak position in Fig.6”, two values 0.75 and 0.84 correspond to two peaks for $T = 0.45$.

T	0.2	0.3	0.35	0.4	0.45
$ \omega_1 $	1.7	1.4	1.2	0.8	0.6
$-\omega_2$	0.08	0.15	0.22	0.30	0.18
$ \omega_L $	1.7	1.4	1.2	0.9	0.6
Peak position in Fig. 4.6	1.68	1.48	1.34	1.14	0.75/0.84

Numerical tests are performed by adding the oscillating external field of

$$H_1 = -h\Theta(t) \cos(\omega_0 t) \cos q$$

with $h = 0.01$. We expect that the system gets larger energy from the external field as frequency ω_0 becomes closer to $\pm|\omega_L|$. Energy gain over time is linear in the theory, and we compute the slope of $U(t)$ in $t \in [0, 100]$ by use of the least mean square method. We selected a short time region to estimate the slope since large energy gain may modify the stationary state f_0 .

The slopes are reported as functions of ω_0 for several values of temperature T in Fig. 4.6. We capture three qualitative features from the slopes: (i) The peak position shifts from right to left as T increases. (ii) The graph for $T = 0.45$ has two peaks and a sign of the double peaks can be observed in the graph for $T = 0.4$. (iii) Height of the peak shows the “V” letter shape as a function of T . Considering the fact that $|\omega_2|$ is much smaller than $|\omega_1|$, and $|\omega_L|$ is close to $|\omega_1|$, the feature (i) directly reflects T -dependence of ω_1 . Similarly, (ii) captures discontinuous change of frequency of the main root around $T \simeq 0.38$, at which two pairs of main roots have the same imaginary part but have different real part. See Fig.11 of Ref. [BOY2010] and Table 4.1 for (i) and (ii). The third feature (iii) may be explained by the maximum work of the external field, which is expressed by Eq. (4.108), and the turn “V” letter shape of $-\omega_2$ as a function of T . See Fig.10 of Ref. [BOY2010] and Table 4.1.

However, the peak position is quantitatively not in agreement with $|\omega_L|$. We introduced two assumptions in the way of deriving the frequency (4.109) giving the maximum work, and they may cause this discrepancy. We remark that this discrepancy, that is the peak positions are slightly larger than $|\omega_L|$ for $T = 0.4$ and 0.45 , is also observed in comparison between the Landau pole and direct numerical computation of frequency in Landau damping by N -body simulations [BOY2010]. We also remark that the energy gain is not completely linear in numerics as shown in Fig. 4.7, and further investigations are necessary to extract non-equilibrium dynamics precisely.

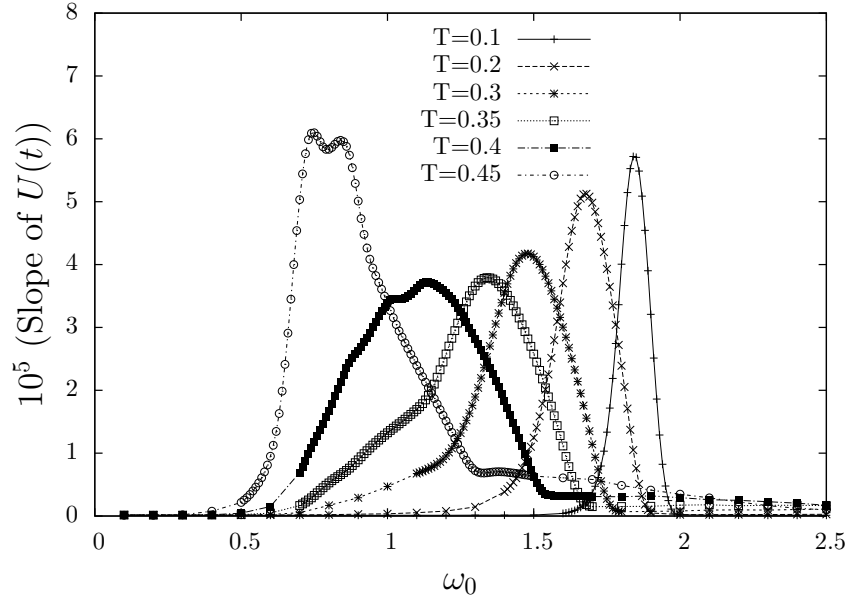


Figure 4.6: Slope of $U(t)$ as a function of ω_0 . The slope is computed by use of the least mean squares method in the time interval $t \in [0, 100]$. Semi-Lagrangian method is performed with $N_q = 128, N_p = 256, \Delta t = 0.05$ and $h = 0.01$.

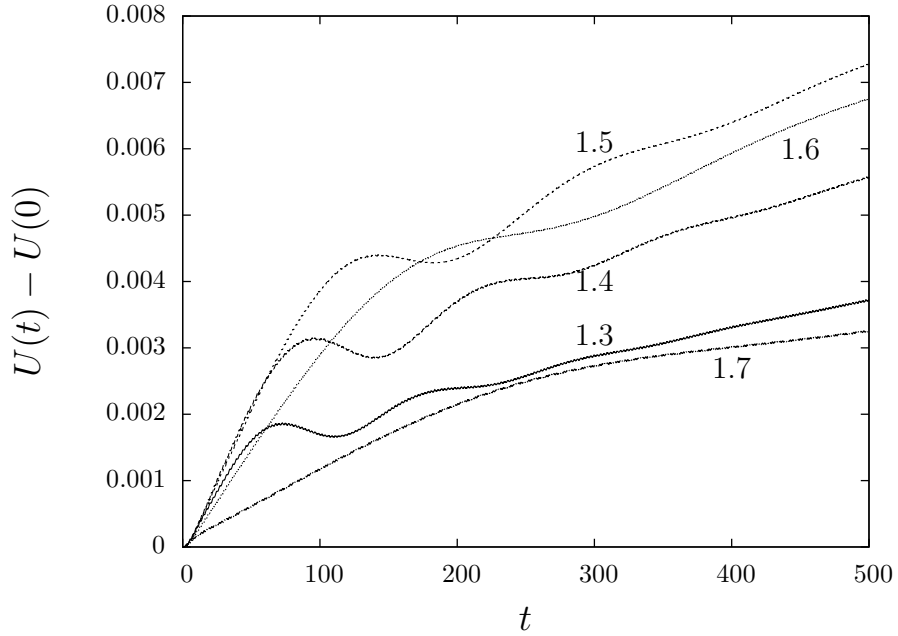


Figure 4.7: Temporal evolution of energy, $U(t) - U(0)$, for some values of ω_0 . $T = 0.3$. The numbers assigned to curves represent ω_0 . Semi-Lagrangian method is performed with $N_q = 128, N_p = 256, \Delta t = 0.05$ and $h = 0.01$.

4.7 Zero-field susceptibility

Let χ_V denote the isolated susceptibility, that is,

$$\chi_V \equiv \frac{1 - D_x(0)}{D_x(0)}, \quad (4.110)$$

and let us rewrite the isothermal susceptibility (2.14) by χ_T . We compare χ_V with χ_T . As we have already seen in Section 4.5.1, the equality

$$\chi_V = \chi_T = \frac{T_c}{T - T_c} \quad (4.111)$$

satisfies in the spatially homogeneous equilibrium states. On the other hand, it is shown that the inequality [OPY2013]

$$\chi_V < \chi_T, \quad (4.112)$$

satisfies in the spatially inhomogeneous equilibrium states. The discrepancy between χ_V and χ_T is evaluated by a Casimir invariant of the Vlasov equation, as for systems obeying Liouville equation [Maz1969] or von-Neumann equation [Suz1971]. This fact is shown by the same procedure with Mazur [Maz1969] (see Appendix C.3).

The inequality (4.112) holds not only for the size of the susceptibilities but also for their critical exponents. The critical exponent γ_-^T of χ_T is $\gamma_-^T = 1$, as we mentioned in Section 2.2. On the other hand, the critical exponent γ_-^V of χ_V is shown to be $\gamma_-^V = 1/4$ [OPY2013]. This exponent is computed from the relation

$$\gamma_-^V = \beta/2 \quad (4.113)$$

and the fact $\beta = 1/2$ (see Section 2.2).

The relation (4.113) is derived as follows: Equation (4.101) and

$$\frac{d\bar{f}_0}{dk}(k) = \frac{2\beta M_0}{\pi I_0(M_0)} \sqrt{\frac{\beta}{2\pi}} k \exp(-\beta M_0(2k^2 - 1)), \quad (4.114)$$

with Eq. (2.15) result in the scaling law,

$$D_x(0) \simeq (T - T_c) + C \sqrt{M_0} \sim \sqrt{M_0} \sim |T - T_c|^{\beta/2}. \quad (4.115)$$

Substituting it into Eq. (4.110), we show the scaling rule (4.113).

We can define the critical exponents β and γ for a one-parameter family of QSSs, where the parameter is, for instance, the energy density U as we have done in Section 4.5, and the family has a second-order phase transition. The value of the exponent β may change due to arbitrariness of the parameterization, but the scaling rule (4.113) holds even for such a family [OPY2013].

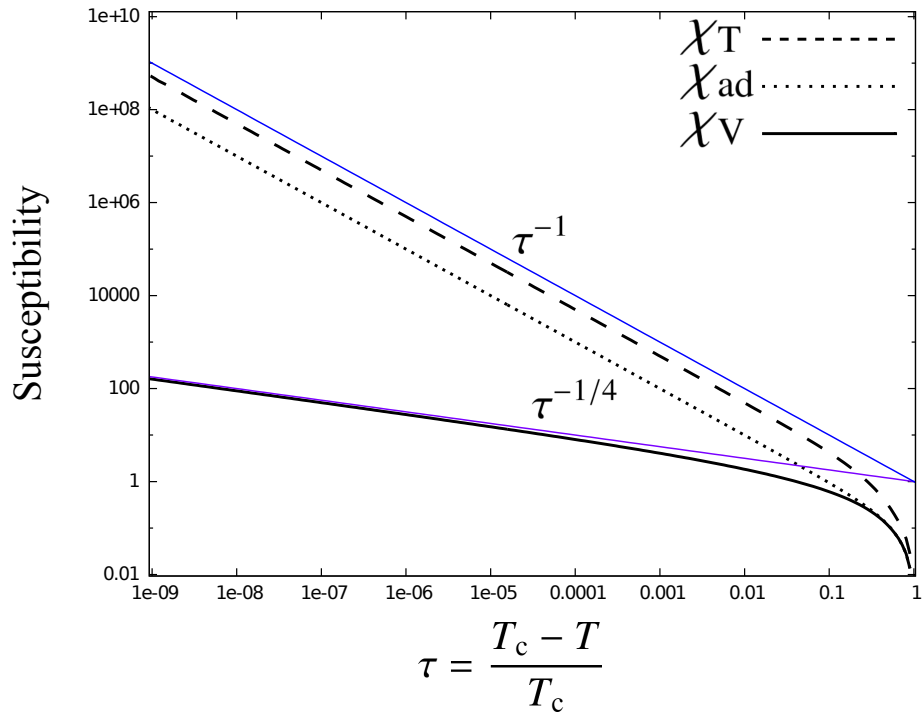


Figure 4.8: The isolated susceptibility χ_v and the isothermal susceptibility χ_T are plotted as functions of $\tau = (T_c - T)/T_c$. The adiabatic (quasi-static) susceptibility χ_{ad} is also plotted, which can be derived by taking the invariance of the entropy under the quasi-static adiabatic process into account.

4.8 Summary and discussion

We have proposed the linear response theory based on the Vlasov equation for spatially periodic one-dimensional Hamiltonian systems. The theory has been examined for homogeneous and for inhomogeneous cases in the HMF model by comparing with direct numerical computations of the Vlasov equation.

As examples of homogeneous distributions, we have considered three families of distributions: thermal equilibrium, power-law tails, and Lynden-Bell distributions. These families have stable or metastable homogeneous states, and such (meta-)stable states become unstable continuously by changing parameters. We hence have expected that the present linear response theory leads a Curie-Weiss like law for the considering families. Indeed, the theory gives the exactly same susceptibility with equilibrium statistical mechanics for thermal equilibrium. The theory also predicts Curie-Weiss like laws even in QSSs of power-law tails and of Lynden-Bell distributions. For the Lynden-Bell distributions, the theory and direct numerical simulations imply that the Curie-Weiss like law holds in an asymptotically high-energy region. The coefficient of the Curie-Weiss like laws tends to be large as momentum deviation of considering homogeneous stationary state becomes large. However, no universality is found in the coefficient as a function of the momentum deviation among the three tested families except for two special points of thermal equilibrium and homogeneous waterbag distribution.

We emphasize that the linear response theory also gives good predictions for the inhomogeneous stationary state. Moreover, the resonance absorption in inhomogeneous thermal equilibrium is useful to investigate non-equilibrium dynamics of an unforced system. Energy gain by oscillating external fields with frequency ω_0 has a peak around $\omega_0 = |\omega_L|$, where ω_L is the main Landau pole, although estimation of the peak position is not complete quantitatively. However, in thermal equilibrium, temperature dependence of ω_L is qualitatively captured by this resonance absorption. Detecting the main Landau pole by use of the resonance absorption may have an advantage against direct computation of roots of dispersion relation, since the latter is a hard task in the inhomogeneous case in particular.

The results obtained for the HMF model are applicable to the generalized HMF model (2.72) when the initial stationary solution f_0 does not depend on the lattice point r and can be written as the function of the effective Hamiltonian $\mathcal{H}_r[f_0](q, p) = p^2/2 - M_0 \cos q$. Let us consider the external field $\vec{h} = (h(r, t), 0)$ such that $h(r, t) = 0$ when $t < 0$, $h(r, t) \rightarrow h$ as $t \rightarrow \infty$ uniformly with respect to r . Since the initial solution f_0 is stable, the dispersion relation $D_x^n(\omega) = 0$ ($n \in \mathbb{Z}$) does not have a root in the upper-half ω plane. By using the same procedure as for the HMF model, the linear response of the order parameter $M_{1,x}$ is shown to be

$$M_{1,x}(t) \rightarrow \frac{1 - D_x^0(0)}{D_x^0(0)} h, \quad t \rightarrow \infty, \quad (4.116)$$

and the zero-field susceptibility is the same with that of the HMF model. Then, we show that the scaling rule $\gamma_- = \beta/2$ [Eq. (4.113)] is true for the generalized HMF model when the site-site interaction $K_N(r)$ satisfies conditions (2.73) and (2.74).

We have neglected the case that the frequency ω_0 of external field coincides with one of branch points of logarithmic singularities in the inhomogeneous case. The logarithmic singularities give algebraic damping of the linear response by the same mechanism shown in Ref.

[BOY2011], though the external forces are exerted eternally. Nevertheless, according to our preliminary numerical test, the algebraic damping could not be observed. This damping may not be robust since (i) we cannot set ω_0 exactly on one of the branch points, and (ii) the branch points are determined by 0-th order stationary state, but may be shifted effectively due to energy gain by the resonance absorption. Detailed analysis of this phenomenon is left for future work.

Chapter 5

Phase diagram and tricritical point for quasi-stationary states in the Hamiltonian mean-field model

5.1 Introduction

The Vlasov dynamics admits continuous infinity of stationary states, and QSSs depend on not only energy but also initial order parameter, for instance. A non-equilibrium statistical mechanics hence must determine a QSS for a given initial non-stationary state. Based on incompressibility of the Vlasov equation and the pioneering work of Lynden-Bell [Lyn1967], a non-equilibrium statistical mechanics has been studied in a plasma system [LPR2008], in gravitating systems [CS1998, LPT2008, Yam2011, JW2011] and in the HMF model [Cha2006, AFB+2007, AFRY2007]. For plasma and gravitating systems the non-equilibrium statistical mechanics is not a complete theory due to appearance of core-halo structure, but it is useful to describe QSSs in the HMF model, though the core-halo structure is also observed in the HMF model [PL2011]. One of the remarkable predictions of the statistical theory is existence of first-order phase transition and a non-equilibrium tricritical point [AFRY2007]. We stress that both the first-order phase transition and the tricritical point never appear in thermal equilibrium of the HMF model. Moreover, around the tricritical point, re-entrant phenomenon to ordered phase has been reported above the critical point [SCDF2009], which is observed by N -body simulations. It is hence worth detecting the tricritical point on a parameter plane accurately, and investigating dynamics around the tricritical point.

The tricritical point has been detected as follows. The non-equilibrium statistical theory gives a Fermi-Dirac type distribution function for a QSS, and the distribution function includes several undetermined variables depending on initial states. The undetermined variables are determined by solving simultaneous equations, which come from conservations holding in the Vlasov equation and the self-consistent condition for potential. After computing values of the undetermined variables, we divide the parameter plane into homogeneous (disordered) phase and inhomogeneous (ordered) phase, and draw transition lines as boundaries of the two phases. The tricritical point is found as the collapsing point between the second-order transition line and the first-order transition line.

Difficulty of detecting the tricritical point comes from complexity of the simultaneous equa-

tions, which include integrals of the Fermi-Dirac type distribution function. One therefore has had to explore the parameter plane by pointwise numerical computations. The tricritical point sensitively depends on accuracy of computations [AFRY2007, SCDF2009], but the accuracy has been improved in a recent work [SCD2011].

Avoiding hard numerical computations to detect position of the tricritical point accurately, we direct our attention to the fact that the order parameter is small enough around the second-order phase transition line, including the tricritical point. This fact admits to expand the simultaneous equations in power series with respect to the order parameter. Truncating simultaneous equations up to fifth order of the order parameter, we can reduce them into one algebraic equation of the order parameter whose coefficients depend on an initial state identified as a point on the parameter plane. The tricritical point is precisely detected by analyzing the coefficients with the aid of Landau's phenomenological theory. This method is much simpler than the method of solving the simultaneous equations used in the previous studies [AFRY2007, SCDF2009, SCD2011]. Around the obtained tricritical point, we revisit the re-entrant phenomenon by performing N -body simulations.

We remark that there are two types of re-entrant phenomenon around the tricritical point. One is predicted by the non-equilibrium statistical mechanics [Cha2006, SCDF2009, SCD2011] by increasing energy with fixing the parameter representing the initial height of waterbag initial distribution. The other is observed numerically and is not theoretically predicted [SCDF2009]. We will focus on the latter type of re-entrant phenomenon by fixing the initial magnetization.

This chapter is organized as follows. We review Lynden-Bell's statistical theory quickly in Section 5.2. The reduction of simultaneous equations is performed in Section 5.3. The reduced equation is analyzed with the aid of Landau's phenomenological theory in Section 5.4. The re-entrant phenomenon is revisited around the tricritical point in Section 5.5. Section 5.6 is devoted to summary and discussions.

5.2 Lynden-Bell statistical mechanics

QSSs are regarded as stable stationary solutions to the Vlasov equation. It is however impossible to predict Vlasov equilibria dynamically for given initial states in general. We then use Lynden-Bell's pioneering idea of statistical mechanics, which takes incompressibility of the Vlasov dynamics into account [Lyn1967]. We consider initial states which are two-valued waterbag distributions expressed by

$$f_{\text{wb}}(q, p) = \begin{cases} f_{\text{I}} & \text{for } (q, p) \in \mathcal{D} \\ 0 & \text{otherwise} \end{cases}, \quad (5.1)$$

$$\mathcal{D} = [-\Delta q, \Delta q] \times [-\Delta p, \Delta p],$$

$$\Delta p \geq 0, \quad 0 \leq \Delta q \leq \pi.$$

The parameter f_{I} is determined by the normalization condition as

$$f_{\text{I}} = \frac{1}{4\Delta q \Delta p}. \quad (5.2)$$

The incompressibility of the Vlasov equation implies exclusivity of area elements having the height f_1 on μ space, and leads the fermionic like entropy [Lyn1967]

$$\mathcal{S}[\bar{f}] = - \iint \left[\frac{\bar{f}}{f_1} \ln \frac{\bar{f}}{f_1} + \left(1 - \frac{\bar{f}}{f_1} \right) \ln \left(1 - \frac{\bar{f}}{f_1} \right) \right] dqdp \quad (5.3)$$

where $\bar{f}(q, p)$ represents the coarse-grained distribution. The derivation of the entropy (5.3) is exhibited in Appendix D.1. In the followings, we drop the bar of \bar{f} for simplicity of the symbol. We stress that the parameter f_1 , which reflects how particles spread in the μ space at the time $t = 0$, appears explicitly in the entropy (5.3), so that the distribution function maximizing $\mathcal{S}[f]$ depends on initial state.

We maximize the entropy (5.3) under the conservations of the normalization condition

$$\mathcal{N}[f] = \iint f(q, p, t) dqdp = 1, \quad (5.4)$$

the total energy condition

$$\mathcal{U}[f] = \iint \frac{p^2}{2} f(q, p, t) dqdp + \frac{1 - (M[f])^2}{2} = U, \quad (5.5)$$

and the total momentum condition

$$\mathcal{P}[f] = \iint p f(q, p, t) dqdp = P. \quad (5.6)$$

By use of Lagrange multipliers, the variational problem is expressed as

$$\delta [\mathcal{S}[f] - \alpha(\mathcal{N}[f] - 1) - \beta(\mathcal{U}[f] - U) - \gamma(\mathcal{P}[f] - P)] = 0, \quad (5.7)$$

and the solution f_{LB} is

$$f_{\text{LB}}(q, p) = \frac{f_1}{1 + e^{\alpha + \beta(p^2/2 - M[f_{\text{LB}}] \cos q) + \gamma p}}. \quad (5.8)$$

From the rotational symmetry of the HMF model, we set $M_y[f] = 0$ and wrote $M_x[f]$ as $M[f]$ without loss of generality.

The distribution function (5.8) has four undetermined variables: the three Lagrange multipliers α, β, γ and the magnetization $M[f_{\text{LB}}]$. The magnetization $M[f_{\text{LB}}]$ must satisfy the self-consistent equation

$$M[f_{\text{LB}}] = \iint f_{\text{LB}}(q, p) \cos q dqdp = M. \quad (5.9)$$

For the waterbag initial state (5.1), the total momentum P takes 0 and hence γ is 0. The distribution function hence becomes

$$f_{\text{LB}}(q, p) = \frac{f_1}{1 + e^{\alpha + \beta(p^2/2 - M \cos q)}}. \quad (5.10)$$

The undetermined parameters α , β , and M are determined by solving three equations (5.4), (5.5) and (5.9) simultaneously for a given initial state parametrized by the pair of $(\Delta q, \Delta p)$. This pair gives the initial magnetization

$$M_{\text{wb}} = \frac{\sin \Delta q}{\Delta q} \quad (5.11)$$

and the energy U

$$U = \frac{(\Delta p)^2}{6} + \frac{1 - (M_{\text{wb}})^2}{2}, \quad (5.12)$$

and hence initial states are also parameterized by the pair of (M_{wb}, U) instead of $(\Delta q, \Delta p)$. We use the former pair.

Solving the simultaneous equations is the most difficult step in determining the distribution function and drawing the phase diagram on the parameter plane (M_{wb}, U) . This is the reason why we need a theoretical reduction of the simultaneous equations.

5.3 Reduction of simultaneous equations

The idea to reduce the simultaneous equations is to expand them into power series of the order parameter M by focusing on the fact that M is small around the second-order phase transition line. The strategy is as follows. We obtain α and β as functions of M by expanding two equations $\mathcal{N}[f_{\text{LB}}] = 1$ and $\mathcal{U}[f_{\text{LB}}] = U$ with respect to M and by solving them up to the fifth order of M . Substituting the obtained α and β into expansion of the equation $M[f_{\text{LB}}] = M$, we have one algebraic equation of M . One solution to the algebraic equation gives one value of magnetization M , and M gives α and β accordingly. The obtained distribution function f_{LB} corresponds to a QSS if it is stable. Roughly speaking, the phase diagram is drawn on the parameter plane (M_0, U) by counting the number of solutions of M .

5.3.1 Elimination of β

We can extract β from integrands of the simultaneous equations by changing variables as $x = p\sqrt{\beta/2}$ and $\eta = \beta M$. The transformed simultaneous equations are

$$f_1\left(\frac{2}{\beta}\right)^{1/2} F(\alpha, \eta) = 1, \quad (5.13)$$

$$f_1\left(\frac{2}{\beta}\right)^{3/2} G(\alpha, \eta) = 2U - 1 + \frac{\eta^2}{\beta^2}, \quad (5.14)$$

$$f_1\left(\frac{2}{\beta}\right)^{1/2} H(\alpha, \eta) = \frac{\eta}{\beta}, \quad (5.15)$$

where the functions F , G , and H are defined by

$$F(\alpha, \eta) = \int_{\mathbb{R}} dx \int_{-\pi}^{\pi} \frac{dq}{1 + e^{\alpha - \eta \cos q + x^2}}, \quad (5.16)$$

$$G(\alpha, \eta) = \int_{\mathbb{R}} dx \int_{-\pi}^{\pi} \frac{x^2 dq}{1 + e^{\alpha - \eta \cos q + x^2}}, \quad (5.17)$$

$$H(\alpha, \eta) = \int_{\mathbb{R}} dx \int_{-\pi}^{\pi} \frac{\cos q dq}{1 + e^{\alpha - \eta \cos q + x^2}}. \quad (5.18)$$

We remark that F and G are even with respect to η , and H odd:

$$\begin{aligned} F(\alpha, -\eta) &= F(\alpha, \eta), \\ G(\alpha, -\eta) &= G(\alpha, \eta), \\ H(\alpha, -\eta) &= -H(\alpha, \eta). \end{aligned} \quad (5.19)$$

The normalization condition (5.13) gives

$$\sqrt{\beta} = \sqrt{2} f_1 F(\alpha, \eta), \quad (5.20)$$

and, using Eq. (5.20), we can eliminate β from energy condition (5.14) and the self-consistent equation (5.15) as

$$F(\alpha, \eta)G(\alpha, \eta) = f_1^2(2U - 1)F(\alpha, \eta)^4 + \frac{\eta^2}{4f_0^2}, \quad (5.21)$$

$$F(\alpha, \eta)H(\alpha, \eta) = \frac{\eta}{2f_1^2} \quad (5.22)$$

respectively.

5.3.2 Determination of $\alpha(\eta)$

We assume that $|\eta| \ll 1$, and solve Eq. (5.21) with respect to α . This assumption requires that both M and β are small, and breaks around $M_0 \simeq 0$ since β becomes large. The solved α , denoted by $\alpha(\eta)$, must be even with respect to η thanks to the fact (5.19). See Appendix D.2 for details. The solution $\alpha(\eta)$ is hence expanded as

$$\alpha(\eta) = \alpha_0 + \alpha_2 \eta^2 + \alpha_4 \eta^4 + \alpha_6 \eta^6 + \dots. \quad (5.23)$$

Substituting the expansion (5.23) into $F(\alpha, \eta)$ we get

$$F(\alpha(\eta), \eta) = F_0(\alpha_0) + F_2(\alpha_0, \alpha_2) \eta^2 + F_4(\alpha_0, \alpha_2, \alpha_4) \eta^4 + \dots, \quad (5.24)$$

where

$$F_0(\alpha_0) = F(\alpha_0, 0), \quad (5.25)$$

$$F_2(\alpha_0, \alpha_2) = F_\alpha(\alpha_0, 0)\alpha_2 + \frac{1}{2}F_{\eta\eta}(\alpha_0, 0), \quad (5.26)$$

$$F_4(\alpha_0, \alpha_2, \alpha_4) = F_\alpha(\alpha_0, 0)\alpha_4 + \frac{1}{2}F_{\alpha\alpha}(\alpha_0, 0)\alpha_2^2 + \frac{1}{2}F_{\alpha\eta\eta}(\alpha_0, 0)\alpha_2 + \frac{1}{4!}F_{\eta\eta\eta\eta}(\alpha_0, 0). \quad (5.27)$$

The symbol $F_{\alpha\eta\eta}$, for instance, denotes that

$$F_{\alpha\eta\eta} = \frac{\partial^3 F}{\partial \alpha \partial \eta^2}. \quad (5.28)$$

The expansion of G is obtained by replacing F with G in the above expressions. Considering Eq. (5.21) in each order of η , we obtain the equations for α_0 , α_2 , and α_4 as

$$F_0G_0 - f_1^2(2U - 1)F_0^4 = 0, \quad (5.29)$$

$$F_0G_2 + F_2G_0 - 4f_1^2(2U - 1)F_0^3F_2 - \frac{1}{4f_1^2} = 0, \quad (5.30)$$

$$F_0G_4 + F_2G_2 + F_4G_0 - f_1^2(2U - 1)(6F_0^2F_2^2 + 4F_0^3F_4) = 0, \quad (5.31)$$

respectively. The value of α_0 is determined by solving Eq. (5.29), which depends on α_0 only. The value of α_2 is determined by solving Eq. (5.30), and we get

$$\alpha_2 = \frac{1 - 2f_1^2(FG_{\eta\eta} - 3F_{\eta\eta}G)}{4f_1^2(FG_\alpha - 3F_\alpha G)}, \quad (5.32)$$

where the functions of the right-hand side are evaluated at $(\alpha, \eta) = (\alpha_0, 0)$. The value of α_4 is computed from the relation

$$\begin{aligned} -F(FG_\alpha - 3F_\alpha G)\alpha_4 = & \left[\frac{1}{2}F(FG_{\alpha\alpha} - 3F_{\alpha\alpha}G) + F_\alpha(FG_\alpha - 6F_\alpha G) \right] \alpha_2^2 \\ & + \left[\frac{1}{2}F(FG_{\alpha\eta\eta} - 3F_{\alpha\eta\eta}G) + \frac{1}{2}F(F_\alpha G_{\eta\eta} + F_{\eta\eta}G_\alpha) - 6F_\alpha F_{\eta\eta}G \right] \alpha_2 \\ & + \left[\frac{1}{4!}F(FG_{\eta\eta\eta\eta} - 3F_{\eta\eta\eta\eta}G) + \frac{1}{4}F_{\eta\eta}(FG_{\eta\eta} - 6F_{\eta\eta}G) \right]. \end{aligned} \quad (5.33)$$

The functions appearing in Eq. (5.33) are evaluated at $(\alpha, \eta) = (\alpha_0, 0)$ again. The solution $\alpha(\eta)$ is hence obtained by Eqs. (5.29), (5.32) and (5.33) up to $O(\eta^5)$.

5.3.3 Reduced equation

Remembering that the function $H(\alpha, \eta)$ is odd with respect to η , we can expand $H(\alpha(\eta), \eta)$ as

$$H(\alpha(\eta), \eta) = H_1(\alpha_0)\eta + H_3(\alpha_0, \alpha_2)\eta^3 + H_5(\alpha_0, \alpha_2, \alpha_4)\eta^5 + \dots, \quad (5.34)$$

where

$$H_1(\alpha_0) = H_\eta(\alpha_0, 0), \quad (5.35)$$

$$H_3(\alpha_0, \alpha_2) = H_{\alpha\eta}(\alpha_0, 0)\alpha_2 + \frac{1}{3!}H_{\eta\eta\eta}(\alpha_0, 0), \quad (5.36)$$

$$H_5(\alpha_0, \alpha_2, \alpha_4) = H_{\alpha\eta}(\alpha_0, 0)\alpha_4 + \frac{1}{2}H_{\alpha\alpha\eta}(\alpha_0, 0)\alpha_2^2 + \frac{1}{3!}H_{\alpha\eta\eta\eta}(\alpha_0, 0)\alpha_2 + \frac{1}{5!}H_{\eta\eta\eta\eta\eta}(\alpha_0, 0). \quad (5.37)$$

Substituting the expansions of F and H , Eqs. (5.24) and (5.34), respectively, into the self-consistent equation (5.22), we obtain the reduced equation in η as

$$\tilde{A}\eta + \tilde{B}\eta^3 + \tilde{C}\eta^5 + O(\eta^7) = 0, \quad (5.38)$$

where

$$\tilde{A} = \frac{1}{2f_1^2} - F_0(\alpha_0)H_1(\alpha_0), \quad (5.39)$$

$$\tilde{B} = -[F_0(\alpha_0)H_3(\alpha_0, \alpha_2) + F_2(\alpha_0, \alpha_2)H_1(\alpha_0)], \quad (5.40)$$

$$\tilde{C} = -[F_0(\alpha_0)H_5(\alpha_0, \alpha_2, \alpha_4) + F_2(\alpha_0, \alpha_2)H_3(\alpha_0, \alpha_2) + F_4(\alpha_0, \alpha_2, \alpha_4)H_1(\alpha_0)]. \quad (5.41)$$

The reduced equation (5.38) is written in η but what we have to compute is a reduced equation in M . For rewriting Eq. (5.38) into the power series of M we expand β as a series of η as

$$\begin{aligned} \beta(\eta) &= 2f_1^2 F(\alpha(\eta), \eta)^2 \\ &= \beta_0 + \beta_2\eta^2 + \beta_4\eta^4 + \dots, \end{aligned} \quad (5.42)$$

where

$$\beta_0 = 2f_1^2 F_0(\alpha_0)^2, \quad (5.43)$$

$$\beta_2 = 4f_1^2 F_0(\alpha_0)F_2(\alpha_0, \alpha_2), \quad (5.44)$$

$$\beta_4 = 2f_1^2 [2F_0(\alpha_0)F_4(\alpha_0, \alpha_2, \alpha_4) + F_2(\alpha_0, \alpha_2)^2]. \quad (5.45)$$

We used the fact that $\beta(\eta)$ is even since $F(\alpha(-\eta), -\eta) = F(\alpha(\eta), \eta)$. Substituting the definition $\eta = \beta M$ into Eq. (5.42) recursively, we get

$$\beta = \beta_0 + \beta_0^2\beta_2M^2 + \beta_0^3(\beta_0\beta_4 + 2\beta_2^2)M^4 + O(M^6), \quad (5.46)$$

and the reduced equation (5.38) is rewritten in the form

$$AM + BM^3 + CM^5 + O(M^7) = 0, \quad (5.47)$$

where

$$A = \beta_0\tilde{A}, \quad (5.48)$$

$$B = \beta_0^2(\tilde{A}\beta_2 + \tilde{B}\beta_0), \quad (5.49)$$

$$C = \beta_0^3[\tilde{A}(\beta_0\beta_4 + 2\beta_2^2) + 3\tilde{B}\beta_0\beta_2 + \tilde{C}\beta_0^2]. \quad (5.50)$$

Note that A , B , and C depend on f_1 and U only, and we can compute their values from a given initial state characterized by (f_1, U) or (M_0, U) . Equation (5.47) is odd with respect to M , and $-M$ is a solution if M is. The number of real solutions is hence 1, 3, or 5 if we neglect $O(M^7)$, and the number depends on signs of the coefficients A , B , and C . For each of the solutions M , values of α and β , and hence the distribution function (5.10), are determined from the expansions (5.23) and (5.42) by using the definition $\eta = \beta M$ up to $O(\eta^5)$.

5.4 Landau's phenomenological theory

It is helpful to introduce the pseudo free-energy $\Psi(M)$, whose critical points represent (meta-) equilibrium states. A critical point of $\Psi(M)$ is stable (resp. unstable) if it is a local minimum (resp. maximum) point. Phase transitions occur when the minimum point of $\Psi(M)$ changes from $M = 0$ to $M \neq 0$. Analysis of phase transitions by using the pseudo free-energy is called Landau's phenomenological theory [LL1968]. For reproducing the reduced equation (5.47) as derivative of the pseudo free-energy, we define $\Psi(M)$ by

$$\Psi(M) = \Psi_0 + \frac{A}{2}M^2 + \frac{B}{4}M^4 + \frac{C}{6}M^6 + O(M^8). \quad (5.51)$$

We note that both $\Psi(M)$ and $-\Psi(M)$ give the same equation for obtaining the critical points, but stability is opposite between the two. The signature of pseudo free-energy is determined by noting that the coefficient A can be rewritten

$$A = \frac{\beta_0}{f_1^2} \left[1 + \pi \int_{-\infty}^{\infty} \frac{1}{p} \frac{df_{\text{LB,hom}}}{dp}(p) dp \right] \quad (5.52)$$

where $f_{\text{LB,hom}}$ is a homogeneous Lynden-Bell distribution function defined by replacing α with α_0 , β with β_0 and setting $M = 0$ in Eq. (5.10). The inside of the brace in Eq. (5.52), denoted by I , represents the spectral [IK1993, Pen1960, CD2009, Oga2013] and the formal stability [YBB+2004] of the homogeneous state $f_{\text{LB,hom}}$, and $I > 0$ (resp. $I < 0$) implies that $f_{\text{LB,hom}}$ is stable (resp. unstable). This fact has been summarized in Section 3.3. The equation $I = 0$ has been used for obtaining the stability diagram of the homogeneous Lynden-Bell distribution function [Cha2006]. From the facts $F_0(\alpha_0) > 0$ and hence $\beta_0 > 0$, the signature of A is identical with I and hence $A > 0$ implies that $f_{\text{LB,hom}}$ is stable. On the other hand, positive A implies that a solution $M = 0$ to $d\Psi/dM = 0$ is a local minimum point, and hence the pseudo free-energy must be $\Psi(M)$ instead of $-\Psi(M)$.

The Landau's phenomenological theory gives phase diagram on (A, B) plane by assuming that C is always positive. The lines $A = 0$ for $B > 0$ and $3B^2 - 16AC = 0$ for $B < 0$ represent second- and first-order phase transition lines respectively. The coexistence region associated to the first-order phase transition is bounded by $A = 0$ and $B^2 - 4AC = 0$. The three lines $A = 0$, $3B^2 - 16AC = 0$ and $B^2 - 4AC = 0$ meet at the origin $A = B = 0$, and the tricritical point is located at the meeting point [NO2011]. We stress that the condition $A = B = 0$ is exact to detect the tricritical point, since five solutions to Eq. (5.47) are degenerated at $M = 0$ irrespective of neglected higher order terms.

The coefficients A and B depend on f_1 and U through α_0 and α_2 , and the phase diagram

on (A, B) plane can be mapped to (M_{wb}, U) plane. We remark that C is always positive around the phase transition lines according to numerical computations. The obtained phase diagram is shown in Fig. 5.1, which is qualitatively consistent with the previously reported one in Ref. [AFRY2007]. We denote the values of U , M_{wb} , and f_I by U^{tc} , $M_{\text{wb}}^{\text{tc}}$, and f_I^{tc} respectively at the tricritical point. The values arranged in Table 5.1 are in good agreement with the values reported in Ref. [SCD2011].

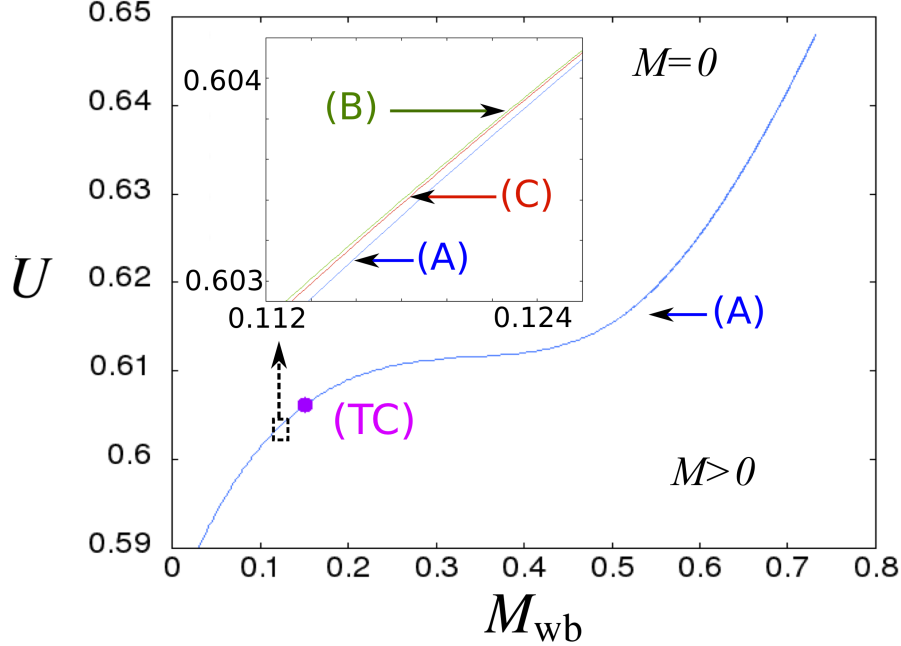


Figure 5.1: Phase diagram on the parameter plane (M_{wb}, U) . Lines (A), (B), and (C) represent $A = 0$, $3B^2 - 16AC = 0$ and $B^2 - 4AC = 0$ respectively. The point (TC) represents the tricritical point. The region enclosed by lines (A) and (B) is the coexistence region. The ordered and the disordered phases appear in the lower side of (B) and the upper side of (A) respectively.

Table 5.1: Comparison of values of parameters at points which are reported as the tricritical point in the present and a previous paper [SCD2011].

	U^{tc}	$M_{\text{wb}}^{\text{tc}}$	f_I^{tc}
Present result	0.606178	0.15118	0.10949
Result in Ref. [SCD2011]	0.6059	0.15	0.109497

5.5 N -body simulations

Results of non-equilibrium statistical mechanics are supported by N -body simulations in a region which is not close to the tricritical point [AFRY2007]. Around the tricritical point, however, a discrepancy between the statistical mechanics and N -body simulations has been reported in Ref. [SCDF2009]. The statistical mechanics predicts monotonically decreasing M as a function of

energy U , but N -body simulations have revealed a re-entrance to inhomogeneous phase in a high-energy region in the (M_{wb}, U) plane. We revisit this re-entrant phenomenon around the obtained exact tricritical point. To avoid confusion, we again stress that this re-entrant phase corresponds to what is called “the second (unexpected) re-entrant phase” in Fig.12 of Ref. [SCDF2009].

The canonical equation derived from the Hamiltonian of the HMF model is written in the form,

$$\frac{dq_i}{dt} = p_i, \quad \frac{dp_i}{dt} = -M_x^N \sin q_i + M_y^N \cos q_i, \quad (5.53)$$

for $i = 1, \dots, N$. We integrate the equation of motion (5.53) numerically by using a fourth-order symplectic integrator [Yos1993] with step size $\Delta t = 0.1$. Initial values of q_i and p_i are randomly drawn from the waterbag distribution (5.1).

We investigate the re-entrant phenomenon by changing value of M_{wb} around the tricritical value $M_{\text{wb}}^{\text{tc}}$. The results of N -body simulations are reported in Figs. 5.2 and 5.3. According to the statistical theory, increasing M_{wb} , the order of phase transition changes from first to second when initial order parameter passes $M_{\text{wb}}^{\text{tc}}$. It is also predicted that the transition energy $U^c(M_{\text{wb}})$ should vary continuously when M_{wb} crosses $M_{\text{wb}}^{\text{tc}}$. This is however not supported by N -body simulations. A schematic picture of energy dependences of magnetization is illustrated for several values of M_{wb} in Fig. 5.4. As M_{wb} increases, the re-entrant phenomenon becomes clearer in one side $M_{\text{wb}} < M_{\text{wb}}^{\text{tc}}$, but it tends to disappear in the other side $M_{\text{wb}} > M_{\text{wb}}^{\text{tc}}$.

To show the signalization of the re-entrance around the tricritical value $M_{\text{wb}}^{\text{tc}}$ clearly, the local maximum and the local minimum, which are observed in panels (b),(c) and (d) of Fig. 5.4, are reported as functions of M_{wb} in Fig. 5.5. The $M_{\text{max}} - M_{\text{min}}$ takes the maximum value around $M_{\text{wb}} = 0.155$, which is close to $M_{\text{wb}}^{\text{tc}}$ within 3% error. This error is compatible with the error of the tricritical point, which is observed by M_{wb} dependence of M with the fixed energy value $U = U^{\text{tc}}$, though it is not reported. We may therefore conclude that the re-entrant phenomenon is signalized around the tricritical point.

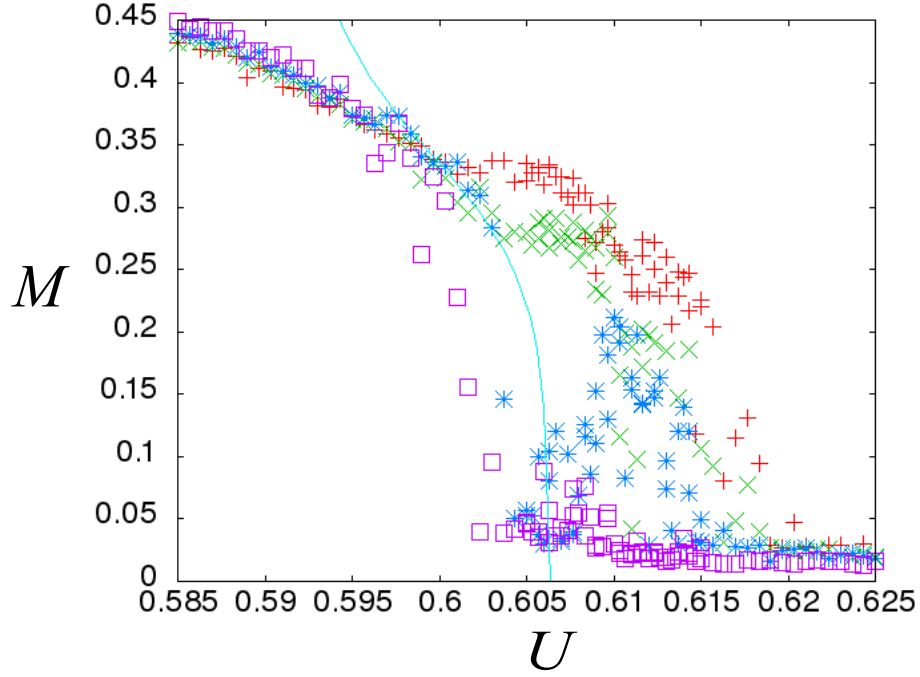


Figure 5.2: Energy dependences of magnetization for four fixed values of M_{wb} around $M_{\text{wb}}^{\text{tc}}$. $M_{\text{wb}} = 0.10(\square)$, $M_{\text{wb}}^{\text{tc}}(\ast)$, $0.18(\times)$, and $0.20(+)$. The number of particles N is 10^5 . Points are obtained by taking averages over time from $t = 500$ to $t = 1000$. The solid line is obtained by using the Landau theory for $M_{\text{wb}}^{\text{tc}}$. We remark that validity of the Landau theory is not guaranteed for large M .

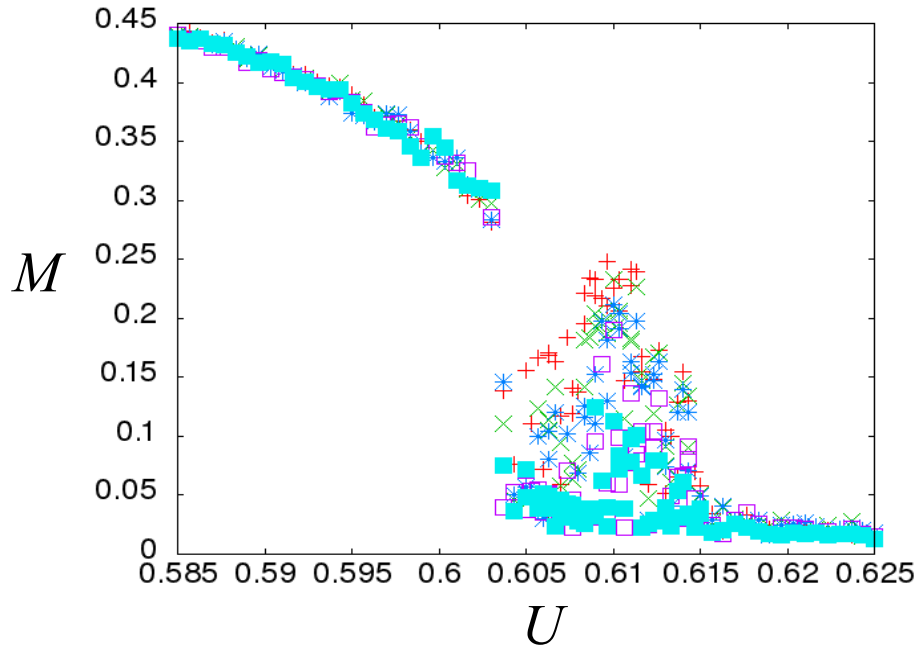


Figure 5.3: The same with Fig. 5.2, but for $M_{\text{wb}} = 0.13(\blacksquare)$, $0.14(\square)$, $M_{\text{wb}}^{\text{tc}}(\ast)$, $0.155(\times)$, and $0.16(+)$.

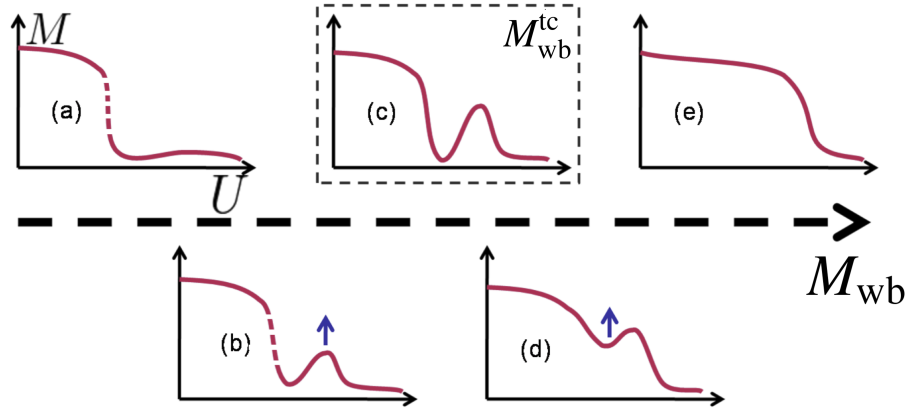


Figure 5.4: Schematic picture of energy dependences of magnetization. Broken lines in (a) and (b) represent jumps due to the first-order phase transitions which are predicted by the statistical mechanics [AFRY2007]. Two upper arrows in (b) and (d) represent direction of change by increasing the initial magnetization M_{wb} . A re-entrant phenomenon appears and grows (b), and the growth stops at the tricritical value M_{wb}^{tc} (c). The panel (d) is for the value of $M_{wb} \sim 0.18$. The re-entrance disappears in large values of M_{wb} (e).

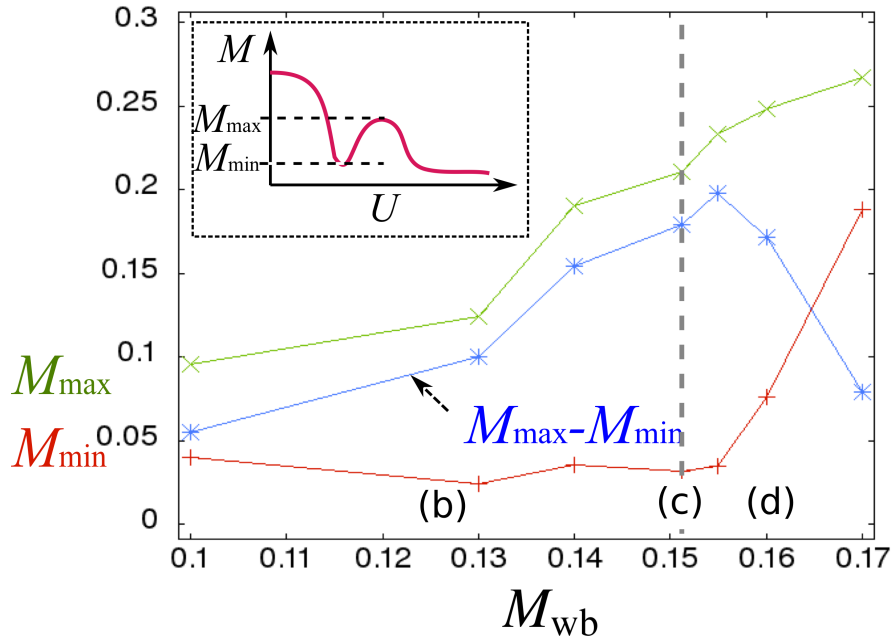


Figure 5.5: The local maximum M_{\max} (\times), the local minimum M_{\min} ($+$), and their difference $M_{\max} - M_{\min}$ ($*$) as functions of M_{wb} . M_{\max} and M_{\min} are defined in the inset. This graph is obtained from the results exhibited in Figs.5.2 and 5.3. The values of M_{wb} marked by (b), (c) and (d) in this figure correspond to panels (b), (c) and (d) of Fig. 5.4 respectively.

5.6 Summary and discussion

A tricritical point has been reported on a parameter plane associated to a family of waterbag initial states in the HMF model. One waterbag initial state goes to a Lynden-Bell distribution, which has three undetermined variables, and the three variables, including the order parameter, are determined by solving three simultaneous equations. Due to difficulty in this solving step, pointwise numerical detection of the position of the tricritical point has been unavoidable.

We have overcome this pointwise detection by deriving one reduced equation for the order parameter by expanding the three simultaneous equations with respect to the order parameter. One solution to the reduced equation gives magnetization in a QSS for a given initial state, which is represented as a point on a two-dimensional parameter plane. The phase diagram on the parameter plane is hence drawn by analyzing the coefficients of the reduced equation, since the coefficients are functions on the parameter plane. We remark that the coefficient of the leading order is equivalent to the formal and linear stability criterion for homogeneous stationary states [YBB+2004, CD2009], and zero level contour of this coefficient corresponds to order-disorder transition. The obtained phase diagram is qualitatively in good agreement with ones previously obtained by directly solving the three simultaneous equations [AFRY2007, SCDF2009, SCD2011]. Furthermore, the tricritical point detected in this chapter is in good agreement with that obtained by the detailed investigation reported in Ref. [SCD2011].

We emphasize that the obtained tricritical point is theoretically exact, since the assumption of the present method is that the product of the order parameter and the inverse temperature is small enough, and is satisfied around the tricritical point. Potential importance of the present method is that it is applicable to other statistical theories and systems, if order parameters explicitly appear in smooth one-body distributions.

One statistical theory has been proposed based on the core-halo structure [PL2011], and the core-halo theory gives a different phase diagram from one given by the Lynden-Bell theory. For applying the present method to the core-halo theory, we need to solve two problems: One is that the core-halo theory includes a parameter determined with the aid of a numerical simulation, and an extended theory is necessary to determine the parameter theoretically. The other is that a distribution function in the core-halo theory is expressed by step functions, which are not smooth and are not expanded in the Taylor series. It might be worth exploring the phase diagram based on the core-halo theory theoretically by overcoming these difficulties.

Around the obtained tricritical point we have revisited the re-entrant phenomenon, which is not a theoretically predicted type [Cha2006, SCDF2009, SCD2011] along iso- f_I lines, but is a numerically observed type [SCDF2009]. The latter type appears even along iso- M_{wb} lines, and we explicitly confirmed the appearance of this type of re-entrance by performing N -body simulations. An important observation by our computations is that the re-entrant phenomenon is signalized around the tricritical point. The origin of this type of re-entrant phenomenon is still unclear, and is an open problem.

Chapter 6

Conclusion and perspective

To summarize this thesis, let us revisit the relaxation process [YBB+2004, BBD+2006, CDR2009] of some systems with long-range interaction, which is reviewed in Chapter 1:

- The system violently relaxes to a QSS.
- In some time scale, such a QSS can be approximately described with a stable stationary solution to the Vlasov equation. The system very slowly relaxes to the equilibrium state due to the finite N effect.

Then, the two limits $N \rightarrow \infty$ and $t \rightarrow \infty$ are incommutable.

- When we take the limit $N \rightarrow \infty$ before taking the limit $t \rightarrow \infty$, the system violently relaxes to a stable stationary solution to the Vlasov equation and it never equilibrate, since there is no finite N effect.
- When we take the limit $t \rightarrow \infty$ before taking the limit $N \rightarrow \infty$, the system is in the equilibrium state.

In this thesis, we have considered the former case. We have centered our interest on the dynamics around given stationary solutions to the Vlasov equation, in Chapters 3 and 4. Further, we have focused on the violent relaxation in Chapter 5.

We have derived the most-refined formal stability criterion [CC2010] and the spectral stability criterion for the inhomogeneous stationary solutions to the Vlasov equation for the HMF model in Chapter 3. These criteria have been found out in the form of necessary and sufficient condition, and have made it possible to decide whether a given stationary solution is possible to be a QSS or not. When the non-zero external field exists, we can discuss the linear stability of the stationary solutions. Our formal stability criterion avoids the problem of finding an infinite number of Lagrange multipliers which has been required in the previously obtained formal stability criterion [CC2010]. We further have shown that stability of some solutions in the family of stationary solutions having two-phase coexistence region in the phase diagram cannot be determined correctly by use of the canonical formal stability criterion which is one of the less refined formal stability criteria [CC2010]. As we have seen in Chapter 5, a family of the Lynden-Bell distributions is one of those families. This fact shows practical usefulness of our stability criteria.

Although the stability criteria have been derived for the HMF model only, it can be straightforwardly applied for the generalized HMF model when a stationary state does not depend on the

lattice point r . Further, for other models, if the dispersion relation is written by the determinant of the block diagonal matrix with small blocks, the most-refined formal stability criterion may be written in an usable form.

Based on the linearized Vlasov equation around the stable stationary solution, the response to the external field in QSSs has been investigated in Chapter 4. In the linear response theory, the dynamics is induced by the unperturbed effective Hamiltonian $\mathcal{H}_0[f_0]$. Such an effective Hamiltonian of the 1D system is completely integrable, so that we can compute the response analytically by using the angle-action coordinates.

We have applied the linear response theory to the HMF model. In the spatially homogeneous QSSs, the theory predicts Curie-Weiss like laws. Further, the isolated susceptibility χ_V coincides with the isothermal one χ_T , when an initial stationary state $f_0(p)$ is the equilibrium state with $T > T_c$. In the inhomogeneous QSSs, the theory suggests the scaling rule $\gamma_-^V = \beta/2$ [Eq. (4.113)] shown in Ref. [OPY2013]. This scaling rule results in $\gamma_-^V = 1/4$ when an initial stationary state $f_0(q, p)$ is the equilibrium state with $T < T_c$. The present linear response theory can be applied to the generalized HMF model (2.72), and this fact may be a supporting evidence of the universality of the scaling rule $\gamma_-^V = \beta/2$.

Further, as application of this linear response theory, we have estimated the Landau poles in inhomogeneous QSSs by use of time-dependent oscillating external fields and the resonance absorption. Detecting the main Landau pole by use of the resonance absorption may have an advantage against direct solving the dispersion relation, since the latter is a hard task in the inhomogeneous case [BOY2010].

Unlike the equilibrium states, QSSs depend not only on conservative macroscopic quantities such as the energy but also non-conservative quantities such as the order parameters in initial non-stationary states. Then, the problem to find a QSS associated with a given initial non-stationary state naturally arises. We however have not gone deep into this problem itself, and have tackle the problem, how we look into the phase transition theoretically when a non-Boltzmann-Gibbs entropy is fixed. The non-equilibrium phase transition based on the Lynden-Bell's statistical mechanics for the HMF model has been discussed in Chapter 5. We have made the Landau's pseudo free-energy from the normalization condition, the energy condition and the self consistent equation. The pseudo free-energy has given us the exact equation to detect the tricritical point, so that we could overcome the pointwise numerical detection of the tricritical point. Although the discussion in Chapter 5 is based on the Lynden-Bell's statistical mechanics, the present method is applicable to other non-equilibrium statistical mechanics theory and other models, if the order parameters explicitly appear in differentiable distribution functions. That is a potential importance of the present method. Some modification is needed to apply this method to the core-halo distribution, since the core-halo distribution is not differentiable [PL2011].

We end this chapter by remarking the application and generalization of the results of this thesis.

Thanks to the fact that all single-body effective Hamiltonians of the 1D systems with stationary solutions are completely integrable, so that we could use the angle-action coordinates [Arn1989] in Chapters 3 and 4. For the long-range interaction system in the higher-dimensional space ($d \geq 2$), in general, it is impossible to apply the use of the angle-action coordinates for investigating linear dynamics around the QSS unless the stationary solution f_0 has symmetry so that the associated effective Hamiltonian $\mathcal{H}[f_0]$ becomes integrable. Generalization to the higher-dimensional system is important in at least two points of view. One is related to basic

motivation to study systems with long-range interaction. An aim of investigation of the statistical physics for such systems is to look into the many body problems in stellar systems and plasmas systems. It is then important to deal with 3D gravitational systems and 3D Coulomb interaction systems, although it can be expected that results obtained via use of the simple models such as the HMF model have some universality. The other is closely related to this thesis. For instance, we have mentioned about the scaling rule between the two critical exponents $\gamma_-^V = \beta/2$ [OPY2013], and we note that this scaling rule holds true for the generalized HMF model (2.72). This generalization has been done for the cite-cite interaction range, but the internal degrees of freedom are still XY-spins. Then, if we can extend our result for the higher-dimensional models, for instance the infinite-range classical Heisenberg like rotators model [NT2003, NT2004] or the classical Heisenberg model with mean-field interaction evolving under the spin dynamics [GM2010], these might be possible to be another supporting evidence of the universality. The ideal solution is sure to find a renormalization group method which has been used in the equilibrium state [NO2011] for QSSs, but it would be hard to imagine.

Meanwhile, the present thesis deals with only classical systems. However, a state similar to the QSS has also been observed in quantum systems [Kas2011, Kas2012], and the quantum HMF model has been studied [Cha2011b, Cha2011c] recently. It might be worthwhile to look into the linear response theory for the quantum long-range interaction systems.

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Appendix A

Elliptic integrals and elliptic functions

We define the complete elliptic integrals and the Jacobian elliptic functions after Refs [WW1927, AS1972, BOY2011]. We first define the Legendre elliptic integrals of the first and the second kinds as

$$F(\phi, k) \equiv \int_0^\phi \frac{d\varphi}{\sqrt{1 - k^2 \sin^2 \varphi}}, \quad E(\phi, k) \equiv \int_0^\phi \sqrt{1 - k^2 \sin^2 \varphi} d\varphi, \quad (\text{A.1})$$

respectively, where the parameter k is the elliptic modulus. The complete elliptic integrals of the first and the second kinds are given by putting $\phi = \pi/2$ into Eq. (A.1) as

$$K(k) = F(\pi/2, k), \quad E(k) = E(\pi/2, k), \quad (\text{A.2})$$

respectively. The Jacobian elliptic functions $\text{sn}(u, k)$, $\text{cn}(u, k)$ and $\text{dn}(u, k)$ are defined respectively so as to be [AS1972]

$$\begin{aligned} \text{sn}(F(\phi, k), k) &= \sin \phi, \\ \text{cn}(F(\phi, k), k) &= \cos \phi, \\ \text{dn}(F(\phi, k), k) &= \sqrt{1 - k^2 \sin^2 \phi}. \end{aligned} \quad (\text{A.3})$$

It should be noted that $\text{sn}(u, k)$ and $\text{cn}(u, k)$ are $4K(k)$ -periodic functions and $\text{dn}(u, k)$ is $2K(k)$ -periodic functions, that is,

$$\begin{aligned} \text{sn}(u + 4K(k), k) &= \text{sn}(u, k), \quad \text{cn}(u + 4K(k), k) = \text{cn}(u, k), \\ \text{dn}(u + 2K(k), k) &= \text{dn}(u, k). \end{aligned} \quad (\text{A.4})$$

It is also remarked that $\text{sn}(u, k)$ is an odd function, and $\text{cn}(u, k)$ and $\text{dn}(u, k)$ are even functions with respect to u . The important relations are summarized as follows:

$$\begin{aligned} \text{sn}(u, k) &= -\text{sn}(-u, k) = -\text{sn}(u + 2K(k), k) = \text{sn}(2K(k) - u, k), \\ \text{cn}(u, k) &= \text{cn}(-u, k) = -\text{cn}(u + 2K(k), k) = -\text{cn}(2K(k) - u, k), \\ \text{dn}(u, k) &= \text{dn}(-u, k) = \text{dn}(2K(k) - u, k). \end{aligned} \quad (\text{A.5})$$

Appendix B

Appendix to Chapter 3

Derivation of the explicit expression of $C^0(J(k))$

We derive the explicit form of $C^0(J(k))$,

$$C^0(J(k)) = \frac{1}{2\pi} \int_{-\pi}^{\pi} \cos q(\theta, J(k)) d\theta. \quad (\text{B.1})$$

Remembering the notation (2.53) and (2.55), and using Eq. (2.51) and the properties of the Jacobian elliptic functions exhibited in Appendix A, we compute $C_\alpha^0(J_\alpha(k))$ for $\alpha = 1, 2, 3$.

For $k < 1$, i.e., $(q, p) \in U_2$, we compute $C_2^0(J_2(k))$ as follows:

$$\begin{aligned} C_2^0(J_2(k)) &= \frac{1}{2\pi} \int_{-\pi}^{\pi} \cos q_2(\theta_2, J_2(k)) d\theta_2 \\ &= 1 - \frac{k^2}{\pi} \int_{-\pi}^{\pi} \text{sn}^2\left(\frac{2K(k)}{\pi}\theta_2, k\right) d\theta_2 \\ &= 1 - \frac{2k^2}{K(k)} \int_0^{K(k)} \text{sn}^2(u, k) du \\ &= 1 - \frac{2k^2}{K(k)} \int_0^{\pi/2} \frac{\text{sn}^2(F(\phi, k), k)}{\sqrt{1 - k^2 \sin^2 \phi}} d\phi \\ &= 1 - \frac{2k^2}{K(k)} \int_0^{\pi/2} \frac{\sin^2 \phi}{\sqrt{1 - k^2 \sin^2 \phi}} d\phi \\ &= \frac{2E(k)}{K(k)} - 1, \end{aligned} \quad (\text{B.2})$$

where we have used Eqs. (A.5), (A.1), and (A.3) to show the third, fourth, and fifth equalities respectively.

For $k > 1$, i.e., $(q, p) \in U_1 \cup U_3$, we compute $C_\alpha^0(J_\alpha(k))$ ($\alpha = 1, 3$) by using the same procedure

in Eq. (B.2) as follows:

$$\begin{aligned}
C_{\alpha}^0(J_{\alpha}(k)) &= \frac{1}{2\pi} \int_{-\pi}^{\pi} \cos q_{\alpha}(\theta_{\alpha}, J_{\alpha}(k)) d\theta_{\alpha} \\
&= 1 - \frac{2}{K(1/k)} \int_0^{K(1/k)} \operatorname{sn}^2(u, 1/k) du \\
&= 1 - \frac{2}{K(1/k)} \int_0^{\pi/2} \frac{\operatorname{sn}^2(F(\phi, 1/k), 1/k)}{\sqrt{1 - k^{-2} \sin^2 \phi}} d\phi \\
&= 1 - \frac{2}{K(1/k)} \int_0^{\pi/2} \frac{\sin^2 \phi}{\sqrt{1 - k^{-2} \sin^2 \phi}} d\phi \\
&= 2k^2 \frac{E(1/k)}{K(1/k)} + 1 - 2k^2.
\end{aligned} \tag{B.3}$$

Appendix C

Appendix to Chapter 4

C.1 Derivation of Eq. (4.14)

The linear response of B is simply written as

$$\langle B \rangle_1(t) = - \iint_{\mu} dq dp B(q, p) \int_0^t e^{(t-s)\mathcal{L}_0} A(q, p, s) ds, \quad (\text{C.1})$$

where

$$A(q, p, t) = \{\mathcal{V}[f_1](q, p, t) + H_1(q, p, t), f_0(q, p)\}. \quad (\text{C.2})$$

We derive Eq. (4.14) from Eq. (C.1).

Let $A_0(q, p)$ be a smooth function, and $A(q, p, t)$ be a solution to the equation

$$\frac{\partial A}{\partial t} + \{\mathcal{H}_0[f_0], A\} = 0 \quad (\text{C.3})$$

with the initial condition $A(q, p, 0) = A_0(q, p)$. Using the linear operator \mathcal{L}_0 , the solution $A(q, p, t)$ is expressed by

$$\begin{aligned} A(q, p, t) &= e^{t\mathcal{L}_0} A_0(q, p) = e^{(t-s)\mathcal{L}_0} e^{s\mathcal{L}_0} A_0(q, p) \\ &= e^{(t-s)\mathcal{L}_0} A(q, p, s). \end{aligned} \quad (\text{C.4})$$

We derive another expression of the solution $A(q, p, t)$ by using a solution of the canonical equation of motion.

Let $(q(t), p(t)) = \phi_0^t(q, p)$ be a solution to the canonical equation of motion

$$\dot{q} = \frac{\partial \mathcal{H}_0[f_0]}{\partial p}(q, p), \quad \dot{p} = -\frac{\partial \mathcal{H}_0[f_0]}{\partial q}(q, p) \quad (\text{C.5})$$

with the initial condition $(q(0), p(0)) = (q, p)$. Equation (C.3) implies that A is constant on this solution and hence

$$\begin{aligned} A(q, p, t) &= A(q(-t), p(-t), 0) \\ &= A(q(-(t-s)), p(-(t-s)), s) = A(\phi_0^{-(t-s)}(q, p), s) \end{aligned} \quad (\text{C.6})$$

holds.

From Eqs. (C.4) and (C.6), we have the relation

$$e^{(t-s)\mathcal{L}_0}A(q, p, s) = A\left(\phi_0^{-(t-s)}(q, p), s\right). \quad (\text{C.7})$$

The above equation rewrites the linear response (C.1) into the form

$$\langle B \rangle_1(t) = - \int_0^t ds \iint_{\mu} B(q, p) A\left(\phi_0^{-(t-s)}(q, p), s\right) dq dp. \quad (\text{C.8})$$

Performing the canonical transform $(q', p') = \phi_0^{-(t-s)}(q, p)$, and using the fact that $\phi_0^{-(t-s)}$ is canonical and $dq' \wedge dp' = dq \wedge dp$ holds accordingly, we have

$$\langle B \rangle_1(t) = - \int_0^t ds \iint_{\mu} B\left(\phi_0^{(t-s)}(q', p'), s\right) A(q', p', s) dq' dp'. \quad (\text{C.9})$$

This equation is nothing but Eq. (4.14), and the derivation is completed.

C.2 Pole singularity of $\tilde{h}(\omega)$

Let $h(t)$ be a smooth function and satisfy

$$\lim_{t \rightarrow \infty} h(t) = h_{\infty}, \quad \text{and} \quad \int_0^{\infty} |h'(t)| dt < \infty. \quad (\text{C.10})$$

We replaced the constant h with h_{∞} to avoid confusion. We prove that the Laplace transform of $h(t)$ is described by

$$\tilde{h}(\omega) = \frac{h_{\infty}}{-i\omega} + \varphi(\omega), \quad (\text{C.11})$$

where all the poles of $\varphi(\omega)$ are in the lower half ω plane.

To prove Eq. (C.11), we show the relation,

$$\lim_{\omega \rightarrow 0} (-i\omega) \int_0^{\infty} e^{i\omega t} h(t) dt = h_{\infty}. \quad (\text{C.12})$$

The proof can be done by integrating by parts as follows:

$$\begin{aligned} -i\omega \int_0^{\infty} e^{i\omega t} h(t) dt &= \left[-e^{i\omega t} h(t) \right]_{t=0}^{\infty} + \int_0^{\infty} e^{i\omega t} h'(t) dt \\ &= h(0) + \int_0^{\infty} e^{i\omega t} h'(t) dt, \end{aligned} \quad (\text{C.13})$$

where we used the condition $\text{Im } \omega > 0$, and $h'(t)$ is the derivative of $h(t)$. Taking the limit $\omega \rightarrow 0$ and using the dominated convergence theorem, we have

$$\lim_{\omega \rightarrow 0} (-i\omega) \int_0^{\infty} e^{i\omega t} h(t) dt = h(0) + \int_0^{\infty} h'(t) dt, \quad (\text{C.14})$$

and this equation proves Eq. (C.12).

To complete the proof of Eq. (C.11), let us check other poles of $\tilde{h}(\omega)$. Suppose that ω_p is a pole. We consider three cases: (i) $\text{Im } \omega_p > 0$, (ii) $\text{Im } \omega_p = 0$ and (iii) $\text{Im } \omega_p < 0$. Performing the inverse Laplace transform, we can reject the cases (i) and (ii) except for $\omega_p = 0$, since the existence of such a pole breaks the condition (C.10). Consequently, Eq. (C.11) has been proved.

Case (iii) is possible, but the contribution from this pole gives an exponentially decreasing term for $M_{1,x}(t)$. We then have shown that the asymptotic value of $M_{1,x}(t)$ is determined by the pole $\omega_p = 0$ when the condition (C.10) holds.

C.3 Derivation of the inequality $\chi_V < \chi_T$

We here use the procedures in the traditional linear response theory. Further we suggest that the methods which have been used in the linear response theory based on the Liouville equation are applicable to the linear response theory based on the Vlasov equation. Such a suggestion might be helpful in future work for other models, although it seems a roundabout way for the HMF model.

To show the inequality $\chi_V < \chi_T$ [Eq. (4.112)], we first show that χ_T and χ_V are written respectively as

$$\chi_T = \frac{\langle C^2 \rangle - \langle C \rangle^2}{T - \langle C^2 \rangle + \langle C \rangle^2}, \quad (\text{C.15})$$

$$\chi_V = \frac{\langle C^2 \rangle - \lim_{t \rightarrow \infty} \langle CC_t \rangle}{T - \langle C^2 \rangle + \lim_{t \rightarrow \infty} \langle CC_t \rangle}, \quad (\text{C.16})$$

where $\langle a \rangle \equiv \iint_{\mu} a f_0 dq dp$, and where $\lim_{t \rightarrow \infty} \langle CC_t \rangle$ is defined as follows,

$$\lim_{t \rightarrow \infty} \langle CC_t \rangle \equiv \lim_{\tau \rightarrow \infty} \frac{1}{\tau} \int_0^{\tau} \langle CC_t \rangle dt = 2\pi \int_L C^0(J)^2 f_0(J) dJ. \quad (\text{C.17})$$

The form of second term in Eq. (C.17) allows us to trace Mazur's procedure [Maz1969]. We note that it is shown straightforwardly that

$$\lim_{\tau \rightarrow \infty} \frac{1}{\tau} \int_0^{\tau} \langle CC_t \rangle dt = \lim_{\epsilon \rightarrow 0+} \epsilon \int_0^{\infty} \langle CC_t \rangle e^{-\epsilon t} dt, \quad (\text{C.18})$$

by using the Abel's theorem [ZMR1997].

Equation (C.15) is obvious, and let us show Eq. (C.16). Let $F_{cc}(t)$ be an inverse Laplace transformation of $\tilde{F}_{cc}(\omega)$ [Eq. (4.59)], then $F_{cc}(t)$ written out as follows

$$F_{cc}(t) = \iint_{\mu} C_t \{C, f_0\} dq dp = -\frac{\langle C \dot{C}_t \rangle}{T}, \quad (\text{C.19})$$

where we have used the fact that $f_0 = A e^{-\mathcal{H}[f_0](q,p)/T}$ and $\dot{C}_t = \{\mathcal{H}[f_0], C_t\}$. Then, $\tilde{F}_{cc}(\omega)$ is written

as

$$\tilde{F}_{cc}(\omega) = -\frac{1}{T} \int_0^\infty \left(\frac{\partial}{\partial t} \langle CC_t \rangle \right) e^{i\omega t} dt = \frac{\langle C^2 \rangle}{T} + \frac{i\omega}{T} \int_0^\infty \langle CC_t \rangle e^{i\omega t} dt. \quad (\text{C.20})$$

Using Eqs. (C.17) and (C.20), we obtain the $\tilde{F}_{cc}(0)$ as follows

$$\begin{aligned} \tilde{F}_{cc}(0) &\equiv \lim_{\epsilon \rightarrow 0+} \tilde{F}_{cc}(i\epsilon) = \frac{\langle C^2 \rangle}{T} - \frac{1}{T} \lim_{\tau \rightarrow \infty} \frac{1}{\tau} \int_0^\tau \langle CC_t \rangle dt \\ &= \frac{1}{T} \left(\langle C^2 \rangle - \lim_{t \rightarrow \infty} \langle CC_t \rangle \right). \end{aligned} \quad (\text{C.21})$$

Equation (C.16) can be shown by using Eq. (C.21), $D_x(0) = 1 - \tilde{F}_{cc}(0)$, and the formula $\chi_V = (1 - D_x(0))/D_x(0)$, [Eq. (4.110)].

Simple derivation of $\chi_V < \chi_T$ We first show the second equality in Eq. (C.17) as follows:

$$\begin{aligned} \lim_{\tau \rightarrow \infty} \frac{1}{\tau} \int_0^\tau \langle CC_t \rangle dt &= \lim_{\tau \rightarrow \infty} \frac{1}{\tau} \int_0^\tau dt \int_L dJ \int_{-\pi}^\pi C(\theta, J) C(\theta_t, J) f_0(J) d\theta \\ &= \lim_{\tau \rightarrow \infty} \frac{1}{\tau} \int_0^\tau dt \sum_{k \in \mathbb{Z}} \int_L 2\pi |C^k(J)|^2 f_0(J) e^{ik\Omega(J)t} dJ \\ &= 2\pi \int_L C^0(J)^2 f_0(J) dJ, \end{aligned} \quad (\text{C.22})$$

since, for $k \neq 0$, the following equation

$$\lim_{\tau \rightarrow \infty} \frac{1}{\tau} \int_0^\tau e^{ik\Omega(J)t} dt = \lim_{\tau \rightarrow \infty} \frac{1 - e^{ik\Omega(J)\tau}}{ik\Omega(J)\tau} = 0 \quad (\text{C.23})$$

is satisfied for almost all J . By use of the third term of Eq. (C.17),

$$2\pi \int_L C^0(J)^2 f_0(J) dJ - \langle C \rangle^2 = 2\pi \int_L (C^0(J) - M_0)^2 f_0(J) dJ > 0, \quad (\text{C.24})$$

for any smooth function $f_0(J)$, since $C^0(J)$ is not constant. From Eqs. (C.15), (C.16), and (C.24), it can be shown that $\chi_V < \chi_T$. It should be noted that

$$\int_L f_0(J) dJ = \frac{1}{2\pi} \iint_\mu f_0(J) d\theta dJ = \frac{1}{2\pi}. \quad (\text{C.25})$$

Mazur's procedure The inequality $\chi_V < \chi_T$ can be also shown by tracing Mazur's procedure [Maz1969]. This procedure seems more complex than the above derivation, but it makes it possible to understand that the difference between two susceptibilities χ_T and χ_V comes from invariants of the dynamics with the effective Hamiltonian $\mathcal{H}_0[f_0]$.

To show the inequality (4.112), we have only to show the equality

$$\lim_{t \rightarrow \infty} \langle CC_t \rangle - \langle C \rangle^2 = \frac{\langle \Delta C Q \rangle^2}{\langle Q^2 \rangle}, \quad (\text{C.26})$$

where $\Delta C \equiv C - \langle C \rangle$, and Q is an appropriate invariant under the dynamics induced by the effective Hamiltonian $\mathcal{H}_0[f_0](J)$. Such an invariant Q is a function of the action J , since it should satisfy $\{Q, \mathcal{H}[f_0]\} = 0$.

We first exhibit a sketch of a proof of the Mazur's inequality [Maz1969]. Let $G(\theta, J)$ be a differentiable function. The inequality

$$\lim_{\tau \rightarrow \infty} \frac{1}{\tau} \int_0^\tau \langle G G_t \rangle dt = 2\pi \int_L G^0(J)^2 f_0(J) dJ \geq 0 \quad (\text{C.27})$$

is satisfied for any function G , where $G^0(J)$ is a zeroth Fourier coefficient of G with respect to θ . Suppose that $\{Q_j(J)\}_{j \in \mathbb{N}}$ is a set of orthogonal functions satisfying

$$\langle Q_j \rangle = 0, \quad \langle Q_i Q_j \rangle = \langle Q_i^2 \rangle \delta_{ij}. \quad (\text{C.28})$$

Putting G as

$$G = \Delta C - \sum_{j \in \mathbb{N}} \frac{\langle \Delta C Q_j \rangle}{\langle Q_j^2 \rangle} Q_j, \quad (\text{C.29})$$

and substituting it into Eq. (C.27), we obtain

$$\lim_{\tau \rightarrow \infty} \frac{1}{\tau} \int_0^\tau \langle \Delta C \Delta C_t \rangle dt - \sum_{j \in \mathbb{N}} \frac{\langle \Delta C Q_j \rangle}{\langle Q_j^2 \rangle} \lim_{\tau \rightarrow \infty} \frac{1}{\tau} \int_0^\tau \langle \Delta C_t Q_j \rangle dt \geq 0. \quad (\text{C.30})$$

By use of the equality

$$\lim_{\tau \rightarrow \infty} \frac{1}{\tau} \int_0^\tau \langle \Delta C_t Q_j \rangle dt = \langle \Delta C Q_j \rangle \quad (\text{C.31})$$

and Eq. (C.17), the inequality (C.30) is arranged in the form of the Mazur's inequality,

$$\lim_{t \rightarrow \infty} \langle C C_t \rangle - \langle C \rangle^2 \geq \sum_{j \in \mathbb{N}} \frac{\langle \Delta C Q_j \rangle^2}{\langle Q_j^2 \rangle}. \quad (\text{C.32})$$

By setting $Q_1(J)$ as

$$Q_1(J) = C^0(J) - M_0 = \frac{1}{2\pi} \int_{-\pi}^\pi \Delta C(\theta, J) d\theta, \quad (\text{C.33})$$

$\langle \Delta C Q_j \rangle = 0$ is satisfied for all $j \neq 1$. Further, the zeroth Fourier mode of G [Eq. (C.29)] vanishes and equalities in Eqs. (C.27), (C.30), and (C.32) are satisfied. The inequality (C.32) is then rewritten in the form of equality

$$\lim_{t \rightarrow \infty} \langle C C_t \rangle - \langle C \rangle^2 = \frac{\langle \Delta C Q_1 \rangle^2}{\langle Q_1^2 \rangle} = 2\pi \int_L \left(C^0(J) - M_0 \right)^2 f_0(J) dJ > 0. \quad (\text{C.34})$$

The last inequality is shown for any smooth function f_0 , since $C^0(J)$ is not a constant. Then, we have shown Eq. (C.26). The inequality (4.112) is derived straightforwardly from Eq. (C.26), and we can conclude that the difference between χ_T and χ_V is completely evaluated with the invariants of the dynamics induced by the effective Hamiltonian $\mathcal{H}_0[f_0]$.

Appendix D

Appendix to Chapter 5

D.1 Coarse-grained distribution and entropy

Any Casimir functionals (2.22) of one-body distribution f are conserved by the Vlasov equation, and so is entropy (5.3). The entropy increasing i.e., the irreversibility, is brought about by a coarse-graining procedure. The coarse-graining procedure has been used to investigate macroscopic properties of both classical and quantum systems. A coarse-graining procedure comes from the limit of ability of our apparatuses in general.

We first divide the μ space into macro-cells, and divide each macro-cell into ν micro-cells. Due to the ability of our apparatuses, we can not detect the difference between $f(q, p)$ and $f(q', p')$ when the point (q, p) and (q', p') are in the same macro-cell. We hence approximate the continuous distribution with the coarse-grained distribution whose range is a finite set $\{\eta_1, \dots, \eta_k\}$, and values are constant in each micro-cells. The coarse-grained distribution $\tilde{f}(q, p)$ is defined as

$$\tilde{f}(q, p) = \sum_{i=1}^k \eta_i \rho(q, p, \eta_i), \quad \eta_i \geq 0, \text{ for } i = 1, \dots, k, \quad \eta_i \neq \eta_j, \text{ for } i \neq j, \quad (\text{D.1})$$

where $\rho(q_r, p_r, \eta_i) \delta q \delta p$ is the probability that the level η_i is found in the r -th macro-cell, $D_r = [q_r - \delta q/2, q_r + \delta q/2] \times [p_r - \delta p/2, p_r + \delta p/2] \ni (q, p)$. The probability ρ is expressed for $(q, p) \in D_r$ as

$$\rho(q_r, p_r, \eta_i) \equiv \frac{(\text{the number of micro-cells filled with the level } \eta_i \text{ in } D_r)}{\nu}. \quad (\text{D.2})$$

The Lebesgue measure of each region which we find level η_i is invariant under the Vlasov dynamics due to the incompressibility, hence the total number of micro-cells filled with the level η_i is conserved ($i = 1, 2, \dots$). It causes the dependences on initial conditions for QSSs.

In this thesis, the range of the coarse-grained distribution \tilde{f} is restricted to be $k = 2$ and $\{\eta_1, \eta_2\} = \{0, f_1\}$. As we mentioned above, the number of micro-cells occupied by the level f_1 is invariant due to the incompressibility. We consider that the initial state is a waterbag distribution,

$$\tilde{f}(q, p, 0) = \begin{cases} f_1 & \text{for } (q, p) \in \mathcal{D}_{\text{ini}}, \\ 0 & \text{otherwise.} \end{cases} \quad (\text{D.3})$$

By the normalization condition, $f_I = 1/|\mathcal{D}_{ini}|$, where $|\mathcal{D}_{ini}|$ is the Lebesgue measure of the region \mathcal{D}_{ini} in the μ space. The parameter f_I reflects how spread elements of the system in the μ space when $t = 0$, and f_I remains explicitly in the distribution function for the QSS.

For deriving entropy, we compute the number of micro states. We call a micro-cell having f_I distribution a particle, which is exclusive and distinguishable. We set the total number of particles is N , and we distribute n_r particles to the macro-cell D_r . The number of ways to this distribution is $N!/\prod_r n_r!$. In each macro-cell D_r , the number of ways to distribute n_r particles into ν micro-cells without degeneracy is $\nu!/(\nu - n_r)!$. The number of micro states is thus

$$W(\{n_r\}) = N! \prod_r \frac{\nu!}{n_r!(\nu - n_r)!}. \quad (\text{D.4})$$

From the Boltzmann's principle and by using the Stirling's formula, we obtain the fermionic like entropy \mathcal{S} written in the form,

$$\mathcal{S} = \ln W = -\nu \sum_r \left[\frac{n_r}{\nu} \ln \frac{n_r}{\nu} + \left(1 - \frac{n_r}{\nu}\right) \ln \left(1 - \frac{n_r}{\nu}\right) \right], \quad (\text{D.5})$$

when we use the unit that the Boltzmann's constant k_B is fixed to 1. By the relation $\bar{f}(q, p)/f_I = \rho(q, p, f_I) = n_r/\nu$ (for $(q, p) \in D_r$) and taking a continuous limit, we obtain the Lynden-Bell's entropy $\mathcal{S}[\bar{f}]$ whose form is,

$$\mathcal{S}[\bar{f}] = - \iint_{\mu} \left[\frac{\bar{f}}{f_I} \ln \frac{\bar{f}}{f_I} + \left(1 - \frac{\bar{f}}{f_I}\right) \ln \left(1 - \frac{\bar{f}}{f_I}\right) \right] dq dp. \quad (\text{D.6})$$

The second term of the entropy comes from the incompressibility of the Vlasov equation.

D.2 Evenness of α

Let us introduce a function $K(\alpha, \eta)$ defined by

$$K(\alpha, \eta) = F(\alpha, \eta)G(\alpha, \eta) - f_0^2(2U - 1)F(\alpha, \eta)^4 - \frac{\eta^2}{4f_0^2}. \quad (\text{D.7})$$

This function K is even with respect to η , and we can expand K as

$$K(\alpha, \eta) = \sum_{n=0}^{\infty} \frac{\partial^{2n} K}{\partial \eta^{2n}}(\alpha, 0) \frac{\eta^{2n}}{(2n)!}, \quad (\text{D.8})$$

where $0! = 1$. We solve $K(\alpha, \eta) = 0$ with respect to α , and show that the solution $\alpha(\eta)$ is even under some assumptions.

We expand the solution $\alpha(\eta)$ as

$$\alpha(\eta) = \alpha_0 + \sum_{m=1}^{\infty} \alpha_m \eta^m. \quad (\text{D.9})$$

Substituting this expansion (D.9) into (D.8), we have

$$K(\alpha(\eta), \eta) = \sum_{n=0}^{\infty} \sum_{k=0}^{\infty} \frac{1}{(2n)!k!} \frac{\partial^{2n+k} K}{\partial \alpha^k \partial \eta^{2n}}(\alpha_0, 0) \left[\sum_{m=1}^{\infty} \alpha_m \eta^m \right]^k \eta^{2n}. \quad (\text{D.10})$$

The condition $K(\alpha(\eta), \eta) = 0$ implies that the coefficient must vanish in each order of η . From the terms of $O(\eta)$, which comes from $n = 0$ and $k = 1$, we get $\alpha_1 = 0$ if $(\partial K / \partial \alpha)(\alpha_0, 0) \neq 0$. The terms of $O(\eta^3)$ are proportional to α_1 or α_3 , and α_3 appears only in the term

$$\frac{\partial K}{\partial \alpha}(\alpha_0, 0) \alpha_3 \eta^3, \quad (\text{D.11})$$

which comes from $n = 0$ and $k = 1$. The coefficient α_1 vanishes and hence $\alpha_3 = 0$ if $(\partial K / \partial \alpha)(\alpha_0, 0) \neq 0$. Similarly, we can prove that $\alpha_{2l+1} = 0$ from the facts that (i) each $O(\eta^{2l+1})$ term includes one odd number of α_m ($m \leq 2l + 1$) at least, (ii) $\alpha_m = 0$ for $m = 1, 3, \dots, 2l - 1$, and (iii) α_{2l+1} comes from $n = 0$, $k = 1$, and $m = 2l + 1$ which gives only the term

$$\frac{\partial K}{\partial \alpha}(\alpha_0, 0) \alpha_{2l+1} \eta^{2l+1}. \quad (\text{D.12})$$

Consequently, if $(\partial K / \partial \alpha)(\alpha_0, 0) \neq 0$ at the $\alpha = \alpha_0$ which satisfies $K(\alpha_0, 0) = 0$, then $\alpha(\eta)$ is even.

The above function $\partial K / \partial \alpha$ is estimated at $\eta = \beta M = 0$, which implies $M = 0$ for finite temperature. Using $M = 0$, the one-body Hamiltonian $\mathcal{H}[f]$ is positive and hence the chemical potential $\mu = -\alpha / \beta$ is positive accordingly. Consequently, the parameter α is negative. Numerical computations reveal that $\partial K / \partial \alpha$ is negative for negative α , and the assumption $(\partial K / \partial \alpha)(\alpha_0, 0) \neq 0$ is satisfied in the HMF model.

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List of author's papers related to this thesis

1. Shun Ogawa and Yoshiyuki Y. Yamaguchi,
Precise determination of the nonequilibrium tricritical point based on Lynden-Bell theory in the Hamiltonian mean-field model,
Physical Review E **84**, 061140 (2011).
 2. Shun Ogawa and Yoshiyuki Y. Yamaguchi,
Linear response theory in the Vlasov equation for homogeneous and for inhomogeneous quasistationary states,
Physical Review E **85**, 061115 (2012).
 3. Shun Ogawa,
Spectral and formal stability criteria of spatially inhomogeneous stationary solutions to the Vlasov equation for the Hamiltonian mean-field model,
Physical Review E **87**, 062107 (2013).
- Chapters 3, 4, and 5 are based on the papers 3, 2, and 1, respectively.
 - Section 2.4 is based on Section V. A and Appendix B of the paper 3.

Figures and tables

Source of figures

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Fig. 2.1 (P. 14) Original.

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Table 4.1 (P. 73) Table 1 of Ref. [OY2012].

Table 5.1 (P. 87) Table 1 of Ref. [OY2011].